WASY Software

FEFLOW® 5.1

Finite Element Subsurface Flow
& Transport Simulation System

User's Manual

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What's new in FEFLOW 5.1

This preface addresses the experienced user who is interested in an overview of the new capabilities of FEFLOW 5.1 compared to the previous release 5.0. Improvements are listed and references to the detailed description of the features in the different FEFLOW manuals are provided. The novice user might skip this section and start with Part I of the manual.

A **newsgroup** has been set up in addition to the online help and different manuals. Look for details at **www.wasy.de/english/service/newsgroups.html**.

The new functions in FEFLOW 5.1 can be divided in following three main parts:

- **model relevant changes**
- **user interface changes**
- **program interface changes**

Model relevant changes

2D variable-density flow and transport modeling with projected gravity field

It allows the 2D density-dependent modeling for confined aquifers by projecting a 3D gravity field onto a horizontal planar model area. A typical application is the transport of brines in thin aquifer layers of sloped geometry (basin). Instead of running a full 3D variable-density flow and transport model, the gravity-projected 2D model option significantly simplifies the computations.

Interface to TRIANGLE mesh generator

An interface to the mesh generator TRIANGLE, copyright© by J. R. Shewchuk (University of California at Berkeley) for complex superelement meshes is integrated. The generator is very fast and especially convenient for superelement meshes which include a large number of add-ins.

Algebraic multigrid solver SAMG

SAMG, copyright© by K. Stüben (FhG-SCAI), allows the efficient solution of large and complex

sparse-matrix systems by the algebraic multigrid method. Special cases involving large parameter contrasts or large number of unknowns can be solved faster by SAMG than by the preconditioned conjugate-gradient iterative solver (PCG). The algebraic multigrid method solves a defined matrix system on a reasonable hierarchy of grids, which is automatically constructed based on the algebraic information explicitly and implicitly contained in the discretization.

Equation solver settings

The equation solver settings can be modified by special dialogs (e.g., iteration stop criterion, maximum iteration numbers).

Geographical transformation

An extended set of geographical transformation methods are provided for superelement meshes and finite-element models. An affine transformation is included in the FEFLOW license as a default method, additional methods, especially for Germany, can be licensed separately.

Transient boundaries and materials

When reducing a transient model to a steady state model, all time-dependent data (boundary conditions, constraint conditions, material properties) are easily reduced to steady-state conditions.

Pathline computation

The existing data sets (transport data and constant value) to derive porosity values for the computation of isochrones were extended. The storativity data set can be used alternatively now.

Variable-density mass transport

The maximum concentration C_s can be modified in the reference mass dialog. Thus the density ratio can be used correctly even if the initial maximum concentration is 0 mg/l.

User interface changes

File-selection dialog

The default Windows file-selection dialog has been implemented in the new version. It replaces the previous Motif-style selection box. Helpful functions such as *Managing of file directories* or *Add favorite directories* are available.

Observation points

Observation points now have properties for labeling and providing drawing attributes. Automatic import and name assignment from `shp`-files is possible. All attributes can be edited and arbitrary points can be deleted interactively. The following import formats have been added: PNT, DXF, SHP, TRP.

Superelement mesh

Edge attributes (linear or parabolic) are saved in the superelement `smh`-file.

Pathline export

Pathline export in 2D and 3D with corresponding attributes (velocities, isochrones) is available in new formats (DXF, SHP, DAT, PNT, PLX, DBF). Additionally, there is a new *Export* button for exporting 3D pathline vertices.

Exporting elemental and nodal quantities

Exporting elemental and nodal quantities and boundary conditions with attributes is possible for a current slice/layer or for all slices/layers.

Fracture elements

The new version 5.1 allows copying of fracture elements for slices in 3D.

Log Messages box

The FEFLOW Log messages box can be easily saved to an arbitrary destination by using the new file selection dialog.

Batch mode

The complete graphical output can be suppressed using batch mode, resulting in faster simulations.

Export of fringed isolines

The export of fringed isolines is available for quadrilateral elements, too.

Automatic regionalization

Automatic assignment of boundary conditions and corresponding constraint conditions (also time dependent) has been implemented. Additionally, the *Join* tool can be used for initial conditions and elevations.

Diagram curves

All curves from diagrams in the simulator (e.g., hydraulic head, flux) are saved in the `dac` file including all time steps. Consequently, important information from the observation points/groups can be fully reconstructed in the postprocessor.

Programming interface

Filter

New filters are available to import superelement meshes or finite element meshes based on `shp`-files, `dxf`-files and `ASCII`-files.

IFM

IFM modules can now integrate Windows dialogs, e.g., using Microsoft Foundation Classes for programming. There are many new API functions for unsaturated flow, for adaptive meshes, for budgeting, and more. The online help gives more information including an exact description of these new functions.

The following table lists the new features which are described in more detail in the FEFLOW documentation and in the online help.

Table: New features in FEFLOW 5.1

Feature	Reference
2D variable-density flow and transport modeling with projected gravity field	White papers Vol. III, Chapter 1
Interface to TRIANGLE mesh generator	User's manual, page 39

Table: New features in FEFLOW 5.1 (continued)

Feature	Reference
Algebraic multigrid solver SAMG	White papers Vol. III, Chapter 3; User's manual, page 23
Equation solver settings	User's manual, page 24
Geographical transformation	User's manual, page 32
Transient boundaries to steady state conditions	User's manual, page 47
Pathline computation	FEFLOW Online Help
Variable density mass transport	FEFLOW Online Help
File selection box	User's manual, page 20
Observation points	User's manual, page 66
Superelement mesh	User's manual, page 32
Pathline export	User's manual, page 17
Fracture elements	User's manual, page 68
Log messages box	User's manual, page 73
Batch mode	FEFLOW Online Help
Diagram curves	FEFLOW Online Help
Filter	FEFLOW Online Help
IFM	FEFLOW Online Help

Part I

Menu Guide

The FEFLOW Shell

1

1.1 Introduction

The graphical FEFLOW *Shell* contains a large amount of commands on several menu levels. Pop-up menus provide additional information. The purpose of Part I is to give a detailed overview of the commands. It can be used as a reference, or it can be perused by users new to FFLOW.

We recommend that you try running FEFLOW before reading past this manual: Please try to perform a first FEFLOW simulation run using the Demonstration Exercise. More information is available from the online **Help** files. Online **Help** is invoked by pressing the **Help** button in some of the menus or by hitting <**F1**>. If a problem cannot be solved by the information found in this manual, you can look in the online **Help** files for additional information. Online **Help** will allow you to quickly and effectively continue your use of FEFLOW.

Some conventions are necessary to clearly describe the *Shell*. This manual contains a section for each command or closely related group of commands. Important pull-down, pop-up, and cascade menus are illustrated. The commands are presented as they would be encountered if you start at the left of the top level menu (*Shell*) and go down each pull-down menu. The explanation continues with the next branch to the right in the *Shell* menu. While running FEFLOW, you can quickly find the reference information of a command by noting the location of the command in the menu structure and finding the corresponding section in this manual. Alternative commands are suggested when appropriate.

1.2 Parts of the Shell

The *Shell* provides a variety of command sequences to formulate and simulate a given problem. It consists of four main parts, which are illustrated in Section Figure 1.1. The working window displays the model with its mesh, boundary conditions, etc., depending on the current operation context. All mouse-based editing is performed here. The shell menu gives access to the different parts and functions of FEFLOW. The menu structure is listed in Figure 1.3. The control panel offers information about the model view and provides tools for zooming and 3D visualization.

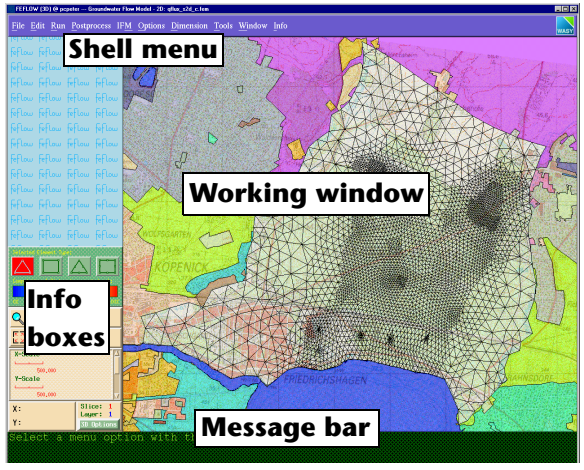


Figure 1.1 Parts of the Shell.

Clicking in the green field which shows the current element type and the progress bar activates the quick-access menu (Figure 1.2) which provides direct access to some of the functions available in the File menu. In the message bar at the bottom of the screen you can find context-sensitive help concerning the operations which you are about to perform, e.g., active hot keys.

Figure 1.2 Quick access menu.

Notice: *The Quick Access menu contains some of the options of the File menu. You can use these options to save data and manage background maps. It is available on every level of FEFLOW by clicking the computational status bar.*

Notice: *You can save edited problem data immediately by clicking the computational status bar in the Quick Access pop-up menu.*

1.3 The Menu Hierarchy

The FEFLOW Shell menu is the top level of a detailed menu structure. The structure is based in part on practical criteria so that basic and often-used settings can be accessed directly from the Shell menu. The lower-level menus follow the sequence of steps of model creation. The basic steps are listed in Table 1.1 together with the corresponding menu names and the sections of this manual that describe them.

Table 1.1 The basic steps of modeling

Topic	Names	Section Number
mesh design	Mesh Editor	Section 3
mesh generation	Mesh Generator	Section 4
attribute specification	Problem Editor	Section 5
simulation	Simulator Run	Section 6
postprocessing	Postprocessor	Section 7

Figure 1.3 The Shell menu with its ten submenus.

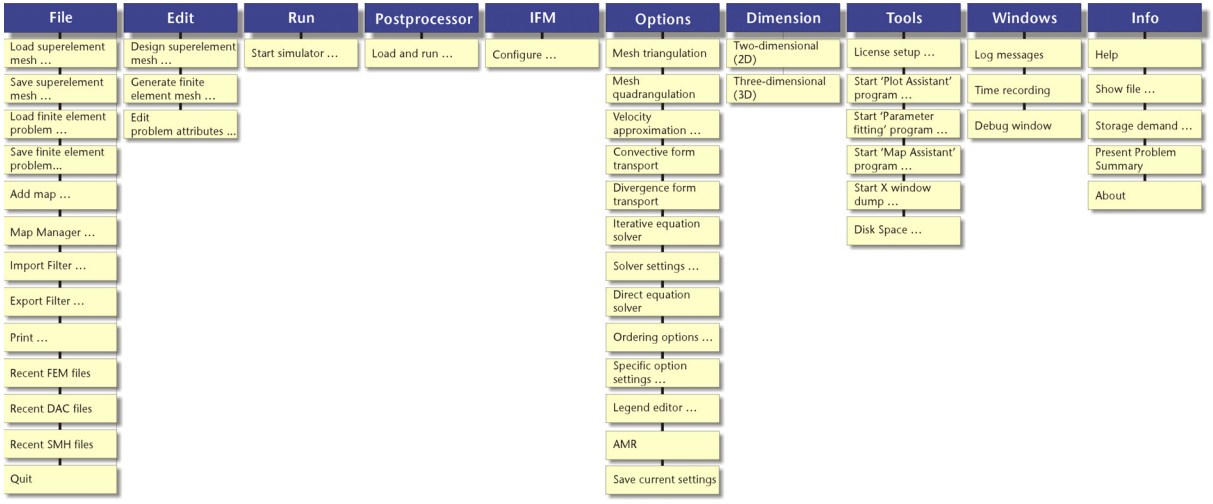


Figure 1.3 FEFLOW Shell menu structure.

1.4 The Zooming Function

The zooming function lets you zoom in and out by dragging a rectangle with the mouse. There is no limiting zoom factor. Activating the button and clicking at any point of interest zooms in with a magnification factor of two. Draw a rectangle with the left or middle mouse button pressed to zoom in or out, respectively.

After activating the button it is possible to move the visible extent of the model with the mouse. The scale of the view is preserved.

The button returns to the previous view extent. For this purpose the last ten view extents are stored. The button resets the view to the default extent

1.5 Display of the Working Window

Additionally to the zooming functions the working window can be adjusted by specifying width and exaggeration of the view. Besides editing the values directly some functions are provided in pop-up menus, which can be invoked by clicking on one of the arrows.

Notice: *Changes in problem width or exaggeration made using the display options affect only the model view. Use the Problem Measure menu to change coordinates or physical extent.*

1.6 The Map Manager

The map manager is a comfortable tool to handle different types of background maps (ASCII point, line and polygon files, ESRI shape files, CAD data and image files). It is opened via the Quick Access Menu or the File menu.

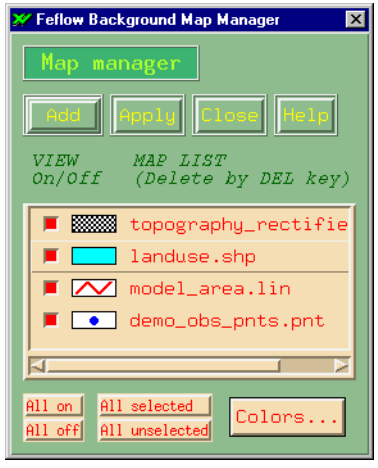


Figure 1.4 Map manager.

For the procedure of adding maps please have a look at the Demonstration Exercise.

In the map manager all currently loaded maps are listed. The uppermost map in the list is shown in the background, whereas the lowest one forms the foreground. At the left side of each map title a small button allows to switch maps on and off for the view. Selecting a map and clicking the Colors button opens the Map ID editor, which offers functionality to set numerous display options for the map. Please note that the following description is only valid for the true-color display mode. For color settings in pseudo-color mode please refer to the FEFLOW online help.

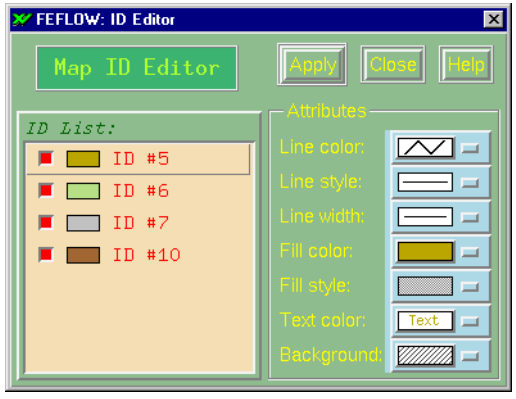


Figure 1.5 Map ID editor.

The left part of the Map ID Editor shows a list of all IDs of the current map. The IDs can be switched on and off for the view using the respective button on the left. If one or several of the IDs have been selected, their properties can be changed in the right part of the window. The seven switches should be self-explanatory, a detailed description can be found in the online help. Note that transparent polygon filling is obtained using the last entry in the Fill style section:

If several IDs have been selected containing different settings for an option, a multi-selection icon is shown:

Click the 'Apply' button to apply the changes.

1.7 The 3D Options Menu

This menu is invoked by clicking the green button in the lower left corner of the working window. The 3D Options menu allows the visualization of a three-dimensional problem as line and fringe drawings for conductivity values, hydraulic head, saturation, moisture content, velocity, mass, or heat distributions. Other options in this menu can be used to cut out parts of the model body for an inside view, to create 3D pathlines, and to visualize isosurfaces. A function to display velocity vectors is also available. See Section 8 and FEFLOW Online **Help** for more detailed information.

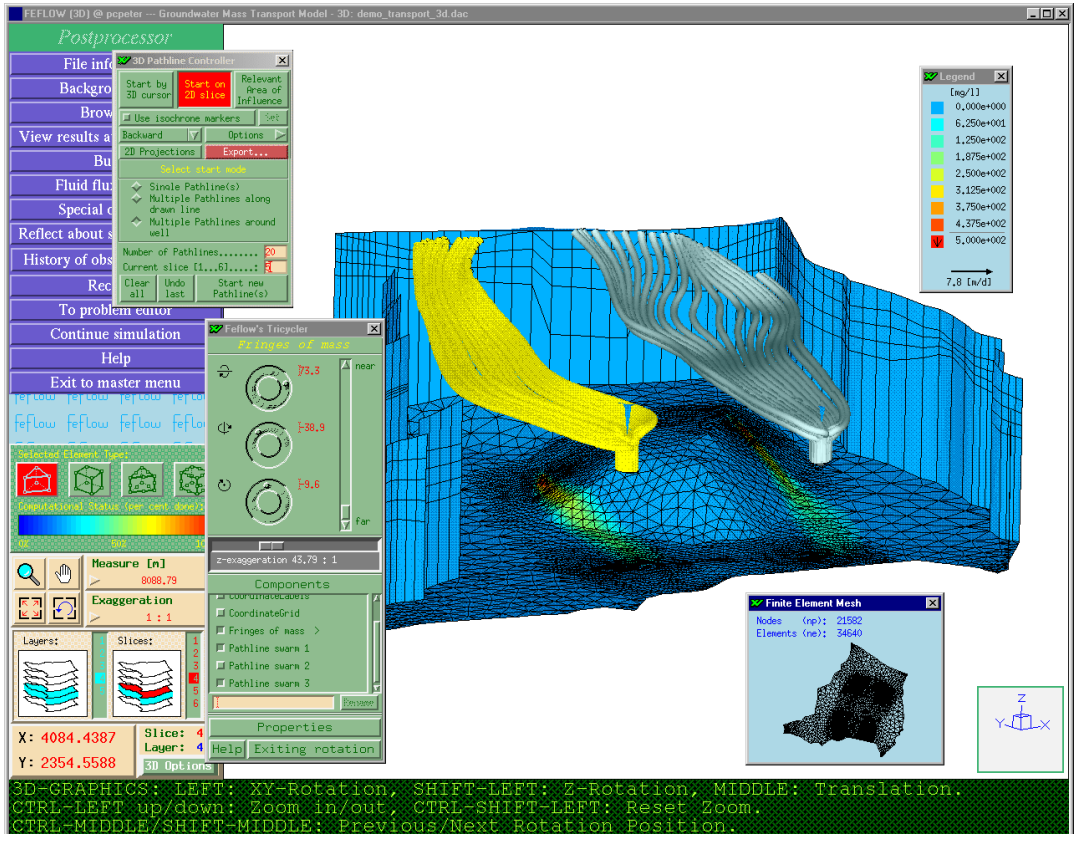


Figure 1.6 The 3D option menu in displaying, for instance, 3D pathlines.

1. The FEFLOW Shell

Shell Menu

2

2.1 Introduction

The FEFLOW graphical *Shell* contains several levels of menu commands. Section 2 describes the top level of the *Shell*. Subsequent sections will cover the lower level commands. Figure 2.1 shows the *Shell* menu.

Figure 2.1 Shell menu.

The following subsections briefly describe the ten submenus: *File*, *Edit*, *Run*, *Postprocessor*, *Options*, *IFM*, *Dimension, Tools, Windows and Info*. The *Quick Access* menu (Figure 2.2) is a pop-up menu containing some *Shell* main-menu items. It is activated by clicking on the green field on the left side of the screen.

All menu and submenu items are selected by clicking the mouse on the item, or by typing the key corresponding to the underlined letter in the item. Inactive menu items are shown in grey. Selecting the menu item in the lowest position of a pull-down menu will often return you to the master *Shell* menu. This allows quick access to other parts of the *Shell* hierarchy.

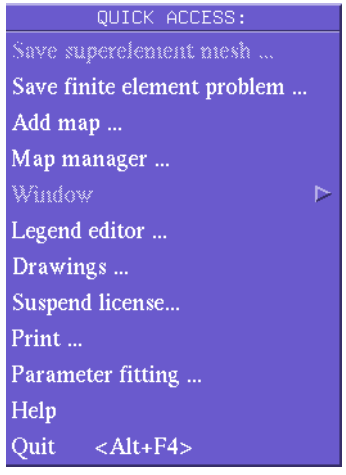
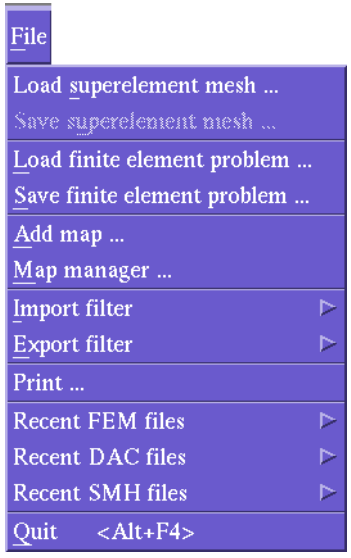


Figure 2.2 Quick access menu.

2.2 File Menu



The **File menu** allows you to load and save all the files necessary for a FEFLOW session. The following paragraphs explain the options in this menu

Load superelement mesh ...

This option loads an existing superelement mesh via the FEFLOW file-selection dialog. It also starts the **Mesh editor**. Figure 2.3 shows the **File selection** dialog that queries you for a filename.

Save superelement mesh ...

Saves the superelement-mesh data you have created.

Load finite element problem ...

Loads an existing finite-element problem by invoking the FEFLOW file-selection dialog (Figure 2.3).

Save finite element problem ...

Saves the complete data for the current finite-element problem. Note that this does not include the superelement mesh.

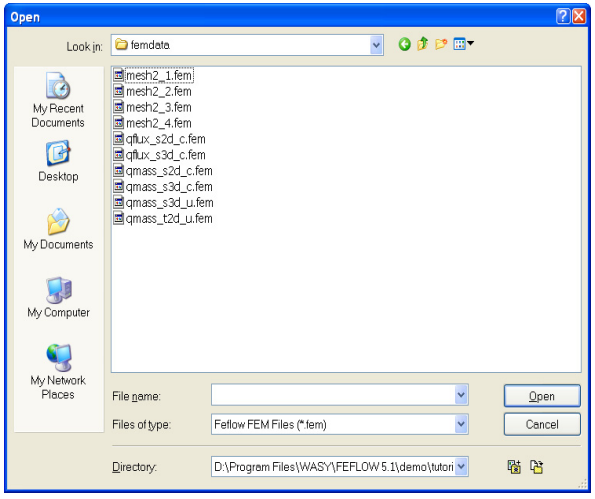


Figure 2.3 FEFLOW file-selection dialog (Windows XP).

The file-selection dialog offers to **Add favorite directories** and to **Manage favorite directories** (Windows operating systems only).

Add map ...

The **Add map** option opens a **File selection** dialog for importing different types of background maps. The list includes: FEFLOW files, Raster Images, HPGL files, ARC/INFO Generate format-files, ArcView compatible shape files, DXF or triplet files.

Map manager ...

This selection opens a submenu for activating or erasing background maps. For detailed information see FEFLOW online **Help**.

Import filter / Export filter

These options manage the loading and saving of data files in additional formats. They are only shown when a folder named 'filter' exists within the FEFLOW home directory. The import of complete data files from the finite-element package Sick 100 is currently supported. The import of superelement meshes is possible in the ASCII Generate Polygon format. All import filters are available on both UNIX and Windows. You can easily add filters for your own data formats. See online **Help** for more detailed information.

Print ... (Windows only)

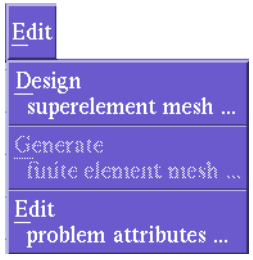
Starts the FEPLOT print tool for automatic visualization of the plot files captured during the current session. The plot files can be saved in FEFLOW on UNIX, too. These files can be subsequently visualized in FEPLOT on a Windows based PC (see also Section 9.1).

Recent FEM/DAC/SMH files

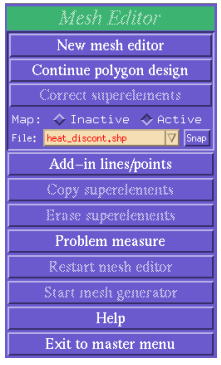
Any of the six most recently used files of each type can be loaded directly from here.

2.3 Edit Menu

This menu is invoked to set up a FEFLOW problem. The following paragraphs explain the commands in this menu:

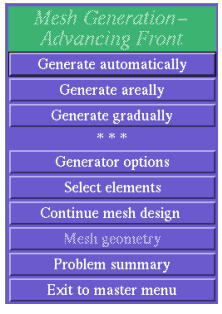


Notice: *The saving options Add map, Map manager, and Print are always available in the Quick Access menu, invoked by clicking on the green field to the left of the working window (Figure 2.2).*



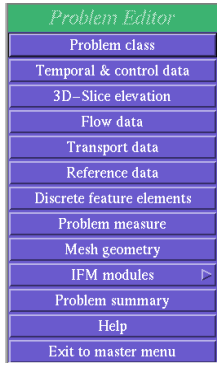
Design superelement Mesh...

invokes the **Mesh editor** for designing a superelement mesh. It uses the mouse (as the basic input environment) or the keyboard. Geometric data for a study area is entered using the FEFLOW **Mesh editor** (see Section 3).



Generate finite element mesh...

opens the **Mesh generator** for creating a finite-element mesh within the designed superelement mesh (see Section 4).



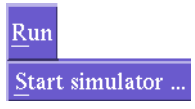
Edit problem attributes...

invokes the **Problem editor** that is used to edit all problem-specific parameters (see Section 5).

2.4 Run Menu

Notice: *Use the Options Menu (Section 2.6) to modify settings for the Simulator Kernel.*

This menu offers the entry to the **Simulation kernel**:



Start simulator...

initializes the FEFLOW **Simulator run** menu which appears to the left of the FEFLOW screen (See Section 6). Note that the **Simulator run** menu is very similar to the **Postprocessor** menu (See Figure 2.4). The simulator's analysis tools like **Budget** or **Fluid flux analyzer** can be applied to the current time step of the simulation, only, while the postprocessor also supports analyzing of time periods.

2.5 Postprocessor Menu

The **Postprocessor** provides capabilities for detailed analysis of simulation results.

Load and run...

loads an output ***.dac** file using the **File-selection** dialog (Section 2.2) and invokes the FEFLOW **Postprocessor** (see Section 7).

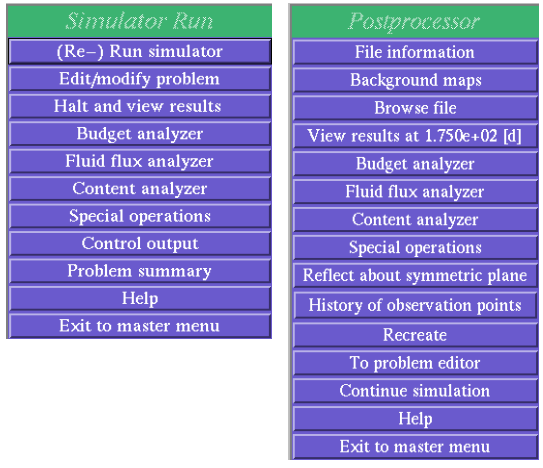
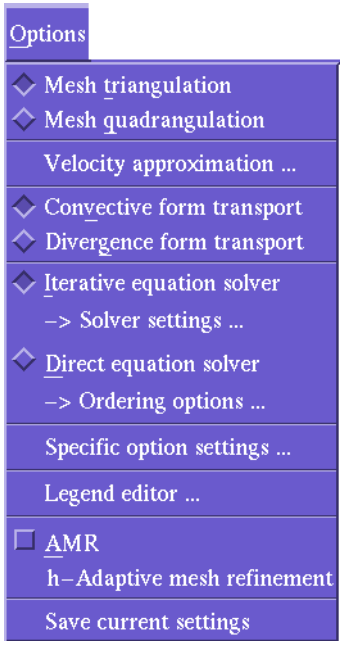


Figure 2.4 Comparison between Simulator Run and Postprocessor menus.

2.6 Options Menu

Many of the items in this menu have default values that are suitable for the novice user.



Mesh triangulation

This (default) setting selects triangular finite elements. Three-nodal or 6-nodal (currently not supported) finite elements are implemented in 2D, and 6-nodal or 15-nodal (currently not supported) prismatic finite elements are available in 3D.

Mesh quadrangulation

selects quadrilateral finite elements. In 2D, you can choose 4-nodal or 8-nodal finite elements. In 3D, the choices are 8-nodal or 20-nodal prismatic finite elements.

Velocity approximation ...

invokes the velocity-approximation options window where a selection of different evaluation methods for the computation of the local Darcy velocities is available.

Convective form transport

applies the default transport equations. These equations are based on the continuity equation to eliminate portions of convective terms, creating a natural dispersive-flux boundary condition. This option is recommended if mass transport can be formulated using first-type boundary conditions and zero dispersive fluxes along the remaining (outflowing) boundary sections.

Divergence form transport

invokes the divergence balance-improved formulation of the governing mass and heat transport equations. This formulation describes a total boundary flux consisting of both convective and dispersive parts. This option is recommended when modeling the total (net) mass or heat flux along inflow boundary sections (e.g. waste injection or leakages from a disposal site, see Reference Manual for details).

Iterative equation solvers

This (default) option is comprised of iterative equation system solvers that are used during the FEM computational process. The symmetric sparse flow equations are commonly solved by a conjugate-gradient method using incomplete Gauss-based preconditioning. As an alternative, FEFLOW also offers the *algebraic multigrid SAMG solver* (separate license required). SAMG has proven very powerful for difficult problems where the conjugate-gradient method takes a large number of iterations (poor convergence) or completely fails (divergence)[1)].

Notice: *The algebraic multigrid solver SAMG is available in FEFLOW for release 5.1 and higher.*

The asymmetric sparse transport equations can be solved by a family of iterative techniques with incom-

[1)] for more see White Papers Vol. III, Chapter 3

plete Crout-based preconditioning. The following solvers are available: Restarted ORTHOMIN, restarted GMRES, CGS, BiCSTAB and BiCGSTABP. BiCGSTABP is the default iterative solver for asymmetric problems. The iterative solvers are very effective and reduce memory requirements. They are efficient for solving large problems containing more than about 20,000 nodes. The maximum iteration number, available preconditioning method and the error criteria can be changed by using the **Properties** dialogs.

Feflow Iterative Solver Settings Menu
Iterative solver settings
Okay
Cancel
Help
NOTICE: Following options applied to the iterative solution of large, sparse matrix equations cover alternative schemes and appropriate parameters which should be carefully selected. They are important for the solution success and influence the storage requirements and the convergence behavior. Change the default options only if be sure!
Available methods for solving symmetric equation systems:
Preconditioned conjugate gradient PCG (Default)
Algebraic multigrid SAMG (by K. Stueben, FhG-SCAI)
Properties ...
Available methods for solving nonsymmetric equation systems (using incomplete factorization (IF) preconditioning):
Preconditioned restarted ORTHOMIN - Orthogonalization-minimization method
Preconditioned restarted GMRES - Generalized minimal residual method
Preconditioned Lanczos CGS - Conjugate gradient square method
Preconditioned Lanczos BiCGSTAB - Bi-conjugate gradient stable method
Preconditioned Lanczos BiCGSTABP (Default) - Postconditioned bi-conjugate gradient stable method
Properties ...

Figure 2.5 Iterative solver settings dialog.

Direct equation solver

The *Direct equation solver* is best for small problems (those with less than about 10,000 nodes). A Gaussian profile solver is used for both flow and transport equations. The Reverse Cuthill McKee (RCM) and, as an alternative, the Multilevel Nested Dissection (MLNDS) nodal reordering schemes are incorporated to minimize the matrix fill-in and the storage demand.

Specific option settings ...

opens a submenu for:

- Handling of the concentration and temperature effects on fluid viscosity and density.
- Processing of multi-layered wells.
- Computation of the mass matrices.
- Quadrature rules to evaluate element integrals.
- Treatment of elements having fallen dry.
- Settings for unsaturated flow.
- Reverse flow field option.

For detailed information see online **Help**.

Legend editor ...

sets the properties for visualization of the modeling results. Besides switching between linear, logarithmic, or custom scales different resolutions are supported. Customized legends can be saved and loaded again.

Adaptive mesh refinement (AMR)

invokes automatic refining and derefining of the finite-element mesh during simulation. The AMR is based on an *a posteriori* error estimation for the spatial discretization. It works currently only for 2D triangular meshes.

Save current settings

Important temporal parameters like file histories, paths, solver settings, numerical options, personal

menu entries are saved immediately and FEFLOW will start with these settings next time.

2.7 IFM - Interface Manager

The Interface Manager controls the configuration of the FEFLOW **Programming interface**. It allows the linking of FEFLOW with third-party software or self-created code. Data can be exchanged for preprocessing, during the simulation run and for postprocessing. The interface allows to create additional submenus and menu entries in the FEFLOW GUI, too. The IFM provides support in all phases of building and maintaining user modules. An assistant guides the initial creation process while the project management dispenses with the need to edit *Makefiles* and others. A callback editor generates the source code for each event you intend to handle. Additional tools and editors complete the module-development environment. The modules are activated in the *Add Modules* menu of the Problem Editor (see Section 5.13). Section 11 of this manual introduces the **Programming interface**.

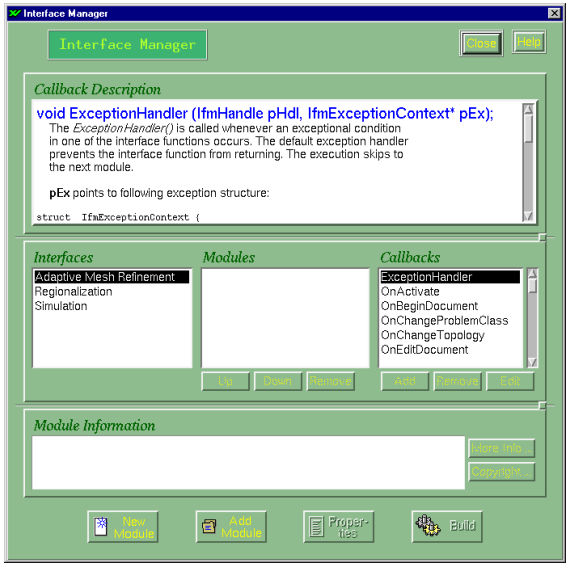


Figure 2.6 Interface manager (IFM).

2.8 Dimension Menu

This menu is used to select the dimensionality of the finite-element formulation.

Two-dimensional (2D)

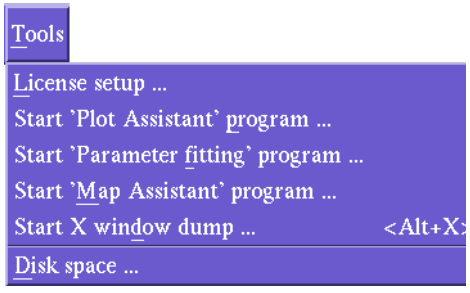
When the 2D toggle is activated, an areal, two-dimensional representation of the study domain and database is used. This default two-dimensional representation covers horizontal, vertical, and axisymmetric models. If invoked for a three-dimensional model, it will reduce the model (including the database) to a single 2D-sliced model representation.

Three-dimensional (3D)

The 3D toggle is activated to employ three-dimensional modeling. If invoked for a two-dimensional model, the model is extended a 3D (multi-aquifer or multi-layer) volume. The extension of the model is controlled by the **3D-Layer Configurator** menu (Section 5.4). This menu immediately appears after the 3D toggle is selected. The **3D-Layer Configurator** menu contains commands to configure the vertical extent of the layer and the geometric relations for a 3D aquifer system.

2.9 Tools Menu

This menu has several submenus giving access to useful programs integrated in FEFLOW.



License setup ...

allows to choose another license server or to add and edit license information for FEFLOW. See the CD-ROM booklet for detailed information.

Start 'Xplot' program ... (UNIX only)

starts the XPLOT plotting program. XPLOT is an X Window-based software tool supplementary to the FEFLOW package. It works interactively to handle all the plotting using the what-you-see-is-what-you-get (WYSIWYG) principle. XPLOT works with the XSPOOL program, another FEFLOW tool. These two programs spool and queue all files directly to a plotter within the UNIX network.

Start 'Plot Assistant' program ... (Windows only)

invokes the sophisticated FEPLOT tool for composing and printing plots based on ESRI Shape files, DXF files and FEFLOW plot files (See Section 6.4.2).

Start 'Map Assistant' program ...

starts a program for georeferencing and rectifying raster images.

Start 'Parameter fitting' program ...

starts the parameter fitting program FE-LM² included with FEFLOW.

Start X window dump ...

opens a small submenu to execute a window dump. Menus or the display of the working window can be dumped and saved in a `.xwd` file. Windows users may prefer to add screen dumps to the clipboard by simply hitting <Alt> + <Print Screen>.

Disk space ...

displays a message window indicating the remaining hard-disk space in the partition containing the current working directory.

2.10 Window Menu

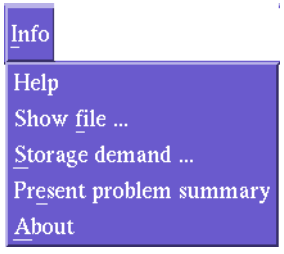
This menu allows you to activate the **Log messages** and the **Time recording** windows for the simulation run. The **Time recording** window reports the CPU and system times needed for each computational step during a simulation run. Normally this option is not set as it is needed only in specific cases. The **Log messages** window lists the error messages and alerts of the program.

The **Debug window** replaces the UNIX console on Windows systems for developing purposes. It is possi-

ble to place messages in this window via interface-manager commands (see Section 11).

2.11 Info Menu

This menu gives an overview over system resources, problem specific information and provides access to the top level of the online **Help** (Section Figure 2.7).



Help

Help invokes the FEFLOW online **Help** pop-up window.

Show file ...

shows (for viewing only) a file to be selected. The FEM output file ***.dar** is the default file type.

Storage demand ...

displays how much memory FEFLOW has allocated for the current model and how much memory will be needed for performing the simulation.

Present problem summary

presents a summary indicating the progress of the editing process. One important item is whether the current problem is ready to run. If it is not ready, you will find hints how to complete the problem. You will also see which parameters have already been user-specified and which parameters have still default values.

About

About opens the **About FEFLOW** pop-up window. It includes copyrights, current version number, the date of the last release, and a disclaimer.

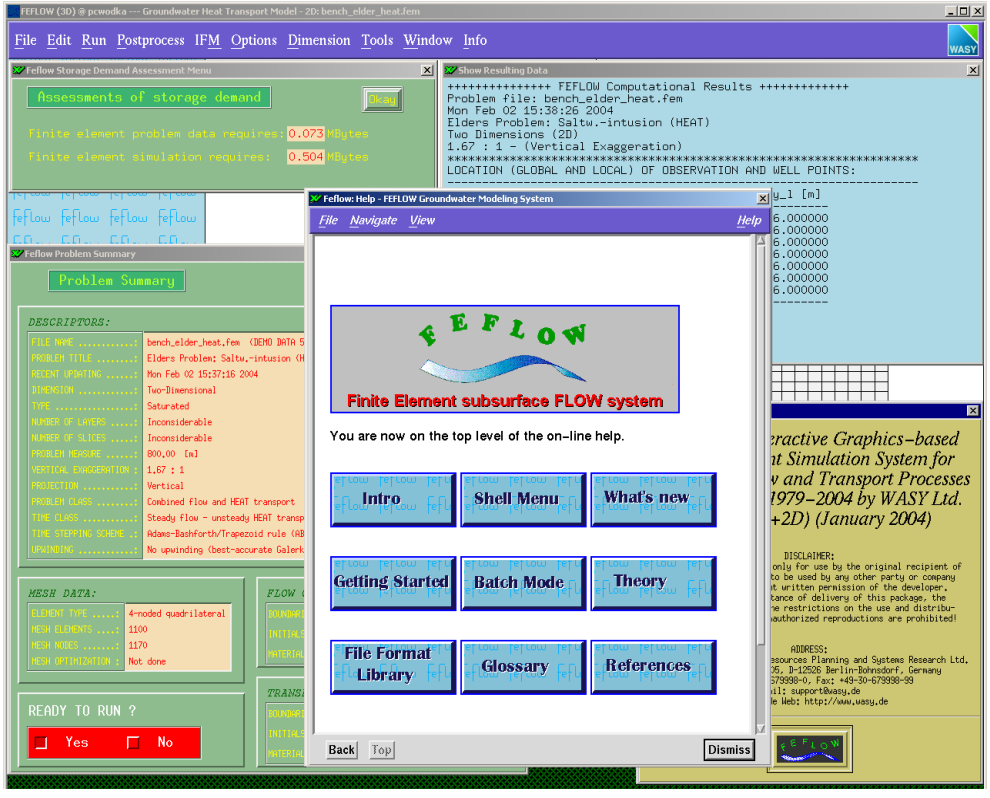


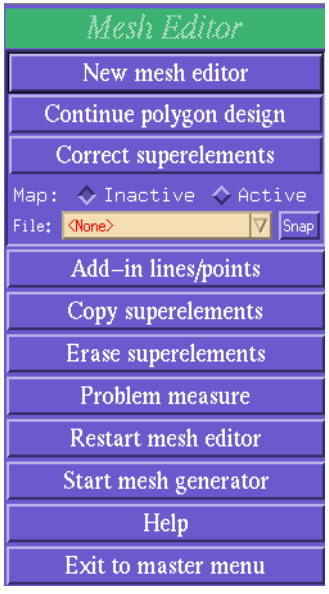
Figure 2.7 Contents of the Info menu.

Mesh Editor Menu Items

3

3.1 Introduction

The **Mesh editor** is a CAD-oriented tool used to enter geometric data for a groundwater flow and transport model. It is the first menu you use when creating a new model. Here you design the superelement mesh which represents the geometry of the study area, i.e., the outer and inner borders of the groundwater model. Superelements are the basis for creating a finite-element mesh.



The **Mesh editor** contains tools to design the superelements. The number of superelements can be arbitrary.

The **Mesh editor** is connected with the **Mesh generator**. The **Mesh generator** is used to interactively mesh superelements with triangular or quadrilateral finite elements. Type and form of the superelements depend on the mesh type selected in the **Options menu** of the *Shell* (Section 2.6).

If you use **Mesh quadrangulation**, you should note that each superelement is automatically closed after the fourth vertex has been set. For **Mesh triangulation** (default), the superelement can have an arbitrary number of vertices, allowing a more complex design.

Superelements are drawn by mouse on a blank screen or on a background map. The keyboard can be used to specify exact coordinates. Meshes or patches of superelements can be easily corrected and manipulated by the following functions and utilities: *Correct*, *Copy*, *Zoom*, *Erase*, *Add*, *Shift*, and *Measure* (for details, see the subsections below). Context-sensitive messages that appear in the message bar help you choose your next step.

Start the Mesh editor:

To Create a New Design: From the **Edit** menu, select **Design superelement mesh ...**. This starts the Mesh Editor with an empty working window.

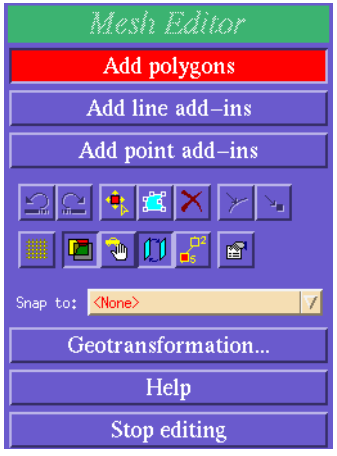
For editing the mesh you can choose between the

mesh editor known up to release 4.8 and the so called 'New mesh editor' which offers more comfortable and more efficient tools for the superelement design.

To Work With an Existing Design: From the **File** menu, select **Load superelement mesh...**. This loads a previously designed superelement data file. You can modify the design in the **Mesh Editor** or you can mesh it by using the **Mesh generator**.

Online **Help** is always available by pressing the **Help** button. Pushing the **Exit to master menu** button returns you to the Master (*Shell*) menu.

3.2 New Mesh Editor



The new mesh editor offers many new capabilities; however, it does not yet include every function available within the old mesh editor. Therefore, both editors are implemented in the current FEFLOW release.

Add polygons

This part of the mesh editor allows you to make changes and additions to a superelement mesh. You can place nodes and change lines to make them curved, circular or straight. For rough orientation the current coordinates of the mouse pointer are shown in the control panel in the lower left corner of the window.

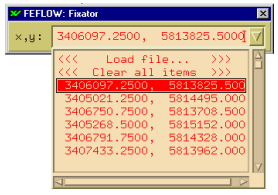


Figure 3.1 Fixator.

Press the left mouse button to fix a node. For exact node positioning the Fixator can be invoked by hitting <F2>. It allows to explicitly enter values for the x and y coordinates of the node. Alternatively, a point file can be loaded by opening the combo box. The points are sorted according to their distance to the mouse pointer. Selecting a point from the list, a new node will be placed exactly at the point coordinates.

After the first superelement node is set, a rubber line that can be dragged is attached to it. The next node is fixed by mouse or keyboard in the same way as the first. Nodes may be created in a clockwise or counter-clockwise direction. Select the starting node again to close a superelement. Before closing the superelement, a recently set node can be clicked again to discard all subsequent nodes. This action is indicated by the cursor. To attach a new superelement to an existing one click one of the existing nodes. Clicking on a superelement edge between vertices inserts a new vertex at the current cursor position. This is indicated by the node-insertion cursor.

During supermesh design it is possible to zoom in and out with the zoomer and to pan the view clicking the middle mouse button and dragging. You can use the <TAB> and <SHIFT>+<TAB> keys for a gradual forward and backward panning, respectively.

Notice: *If you use mesh quadrangulation, each superelement has to be quadrilateral. The superelement is automatically closed after specifying the forth vertex.*

Notice: *Overlapping superelements cause an invalid mesh generation. When using triangular meshes, overlapping of superelements is not automatically prevented. Be sure to check your superelement mesh accordingly.*

Add line add-ins / Add point add-ins

Add-ins specify where nodes are to be set during the finite-element mesh generation. They are very useful, for example, to place nodes exactly at the locations of wells and observation points, or for refining of zones along rivers or faults. Add-ins are only applicable for triangular meshes using the TMesh or the (external) Triangle mesh generator (See Section 4.5). Add-ins are designed in the same manner as superelement polygons.

To add a line add-in draw a line on the screen. The method is identical to the **Add polygons** command. To finish the drawing double-click the left mouse button. The line can start or end inside or outside of the superelements. The parts lying outside of the superelement mesh will be ignored during the mesh generation.

On each node of an add-in line a finite-element node will be created during mesh generation. Options for mesh refining along these lines are available (Section 4.5).

To add point add-ins draw points on the screen or use the Fixator by hitting <F2>. On each point a finite-element node will be created during the mesh generation. Options for mesh refining around these points are available (Section 4.5).

Direct import of points or lines from background maps is currently only supported by the old mesh editor (Section 3.5).

Tools and settings

The new mesh-editor tools and settings are listed in Table 3.1. While most of them are self-explanatory, some will be explained in more detail. The different snapping functions allow an exact positioning of superelement nodes without having to explicitly enter the coordinate values. In the 'Snap to raster nodes' mode the nodes are snapped to the nodes of a regular raster. The raster distance can be set using the 'Editor properties' button.

Table 3.1 Buttons of the New Mesh Editor

Undo	Unlimited undo memory
Redo	Unlimited redo memory
Move nodes	Mode to move single nodes
Select elements	Select elements by mouse-click
Delete	Delete selected elements
Snap to line	Snap nodes to lines
Snap to point	Snap nodes to points
Snap to raster nodes	Snap nodes automatically to (magnetic) raster
Opaque/transparent	Switch display mode for superelements
Auto pan	Automatic panning while editing elements
Node info	Display node and element number
Editor properties	Edit pan, snap, and raster options

Alternatively, a background map loaded using the map manager (Section 2.2) can be used as a template for the superelement generation. Using 'Snap to', the active map can be selected for snapping. Set the corresponding buttons to snap superelement nodes to lines

and/or points of the background map. The snap distance can be changed within the 'Editor properties' window.

Using the 'Move nodes' mode you can correct your superelements by dragging a node while pressing the left mouse button. The Fixator is available by hitting <F2> to specify exact coordinate values. To insert a new node along the edge of an existing superelement, click the left mouse button while the cursor shows the node-insertion symbol . To delete a selected node hit the <DELETE> key. Snapping nodes together closes gaps between different superelements. To separate connected superelements select a shared node and hit <F5>. Curved boundary sections can be created by dragging the middle node (smaller quadrilaterals) of a superelement boundary line. Simultaneous hitting of <F4> creates circular boundaries. Selecting the middle node and hitting <F3> resets the curves to straight lines.

The edge attributes (linear or parabolic) are saved to the supermesh file.

Geotransformation

FEFLOW provides an interface to different geographical transformation routines. FEFLOW comes by default with an affine transformation algorithm in *x*-, *y*- and *z*-directions. The corresponding input dialog appears under the **Transform mesh** submenu of the **Mesh geometry** menu. The target system and the transformation parameters can be defined in a separate dialog after clicking the **Options** button.

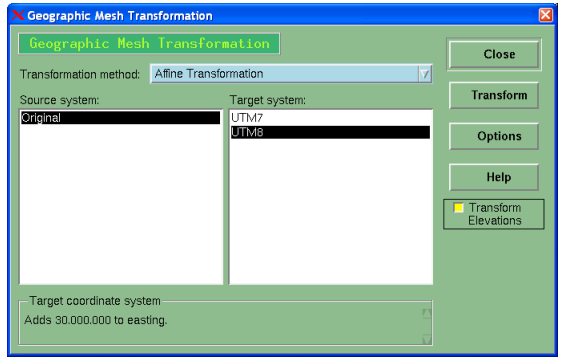


Figure 3.2 Mesh transformation dialog.

Additional methods, especially for Germany, are available and can be licensed separately. Alternatively, it is possible for each user to develop his own transformation routines. In case of need, contact WASY for further information.

3.3 Continue Polygon Design

This part of the old **Mesh editor** allows you to make changes and additions to a superelement mesh. You can place nodes and change lines to make them curved, circular or straight just as described for the new mesh editor. However, there are some differences compared to the New Mesh Editor, e.g., it is not possible to zoom or pan the mesh during the mesh-creation process.

3.4 Map: Inactive/Active

This item allows to use background maps loaded by the map manager (Section 2.2) as templates for the polygon design. Once a file is selected its name is displayed in the "*File:*" text field. The map is activated by setting the toggle to **Active**. During polygon design, the cursor will then snap automatically to items of the background map that are within snap distance. The snap distance can be specified via the **Snap** button next to the **Insert** button. By hitting the <F65> and <F6> keys, the map can be made active and inactive, respectively.

3.5 Add-In Lines/Points

Clicking on the **Add-In lines/points** menu item enters the **Mesh Add-in** submenu. The functionality of add-ins is described in detail in Section 3.2. The commands are described briefly in this section.

Add from map

Imports lines or points from an activated background map:

Having activated a background map as described in the last section the 'Add from map' button becomes enabled displaying 'Add lines from map' or 'Add points from map' depending on the current setting. You can import the corresponding objects all at once by pressing the 'Add from map' button.

Erase add-ins

This option works exactly like the "Erase superelements" (see Section 3.7) function of the Mesh Editor menu.

Help

Starts the FEFLOW Help Viewer for context-sensitive help.

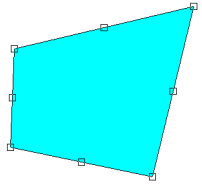
Continue mesh design

Returns to the Mesh Editor menu.

3.6 Copy Superelements

You can copy superelements by translation, rotation, or reflection. Copying can save you time and allows to preserve some properties from one element to the next. Several steps are necessary to copy a superelement. The **Copy superelements** editor will guide you during the process.

Select a superelement or a group of superelements with the left mouse button. The selected superelements are highlighted in light blue on your screen (Figure). You can deselect an element by clicking it again.



Confirm the selection by clicking the right mouse button.

A pop-up window (Figure 3.3) allows you to select between the types of copying *Copy by translation*, *Copy by rotation*, and *Copy by reflection*. Other options in this menu are: *Save original superelement*, *Delete original superelement*, and *Pixel tolerance*. This last option allows you to merge superelements easily. Note that in Figure 3.3 the default toggle buttons are set.

Follow the instructions for the type of copying you have selected.

Copy by translation

Set two points (P1 and P2) for the translation vector.

Copy by rotation

Set the point of rotation axis. Type the angle in degrees for a counterclockwise (positive values) or clockwise (negative values) rotation.

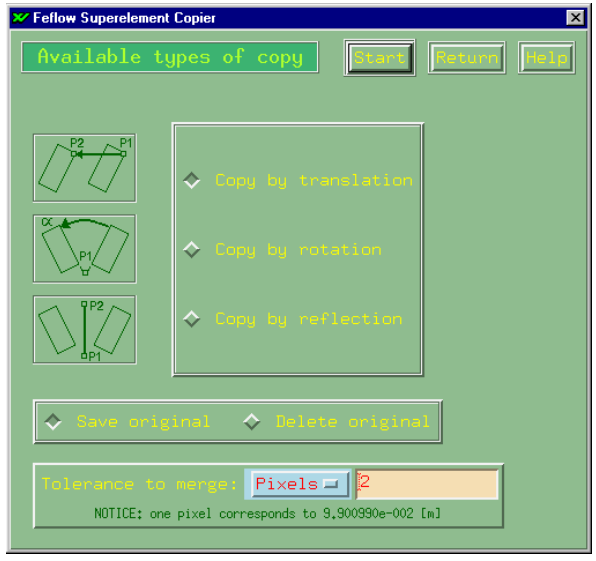


Figure 3.3 Copy superelements.

Copy by reflection

Set two points to mark the reflection line (nodal lassos are operating around marked nodes).

You can discard your newly created supermesh at any time by hitting the <**F2**> key. Return to the first step to repeat a copying procedure or to use a different copy method. To exit the **Copy superelements** mode, press the right mouse button.

3.7 Erase Superelements

Superelements can be erased either individually or collectively. Click on the **Erase superelements** button and select one superelement or a group of superelements with the left mouse button. The selected superelements are highlighted in light blue on your screen. Unselect a previously selected element by clicking it again with the left mouse button. Confirm deleting of the selection with the right mouse button. To undo the erasing of a superelement or a group of superelements hit the <**F2**> key. Exit by clicking the right mouse button.

3.8 Problem Measure

This menu allows to view and edit the dimensions of the working window, the mesh, or the coordinates. Be careful using this menu as the georeferencing of your model is affected by these settings. For invoking the menu click on the **Problem measure** button. A pop-up window appears with the following options:

Width of working window

Sets the width (in meters) of the working area. The default value is 100 m.

Vertical exaggeration

Sets the vertical exaggeration of the working area. The default ratio is 1:1 (no exaggeration).

Shift origin

Displays a toolbar for setting the location of the local coordinate origin:

See Table 3.2 for a detailed description of the toolbar buttons.

Table 3.2 Buttons of the Shift Origin toolbar

Shift origin	Allows to interactively shift the local origin. Move the cross hairs by mouse to any point inside or outside the model area.
Snap origin to (X, Y) coordinates	Origin of local coordinates snaps automatically to a point selected by mouse-click.
Shift origin to lower left corner	Shifts the origin of local coordinates to the lower left corner.
Shift origin to lower right corner	Shifts the origin of local coordinates to the lower right corner.
Shift origin to upper left corner	Shifts the origin of local coordinates to the upper left corner.
Shift origin to upper right corner	Shifts the origin of local coordinates to the upper right corner.
Finish	Exit/close origin tool menu and return to the *Problem measure* menu.

Gauss-Krueger coordinates input

Allows to enter absolute Gauss-Krueger coordinate values, *xoGK* and *yoGK* (in meters), for the origin of the local coordinates. The default values are (0., 0.). You can georeference the working window automatically by importing a background map for the model area (See Section 2.2).

3.9 Restart Mesh Editor

This function should be used only if you wish to discard what you have created with the **Mesh editor**. Before restarting the mesh design, an alert box prompts for a selection from the following options:

- **Save** the current superelement mesh in a file.
- **Restart** the editor from the beginning.
- **Cancel** (no restart).

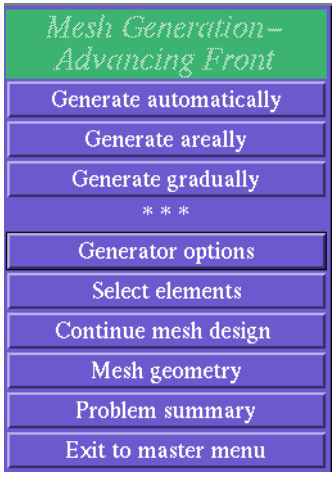
3.10 Start Mesh Generator

Clicking this button opens the **Mesh generator**. The Mesh Generator, which meshes the superelements with finite elements (quadrilaterals or triangles), is discussed in Section 4.

Mesh Generator Menu Items

4

4.1 Introduction



This section describes the generation of finite-element meshes. It is assumed that you have already created one or more superelements. During the simulation, results are computed on each node of the finite-element mesh and interpolated within the finite elements. The denser the mesh the better the numerical accuracy, and the higher the computational effort. Numerical difficulties can arise during the simulation if the mesh contains too many highly distorted elements. Thus some attention should be given to the proper design of the finite-element mesh. To assist in creating a well-shaped mesh, FEFLOW offers various tools, including local refinement and derefinement of the mesh.

4.2 Generate Automatically

A pop-up window allows you to enter the desired total number of finite elements (default is 1000) for the complete region of superelements.

4.3 Generate Areally

Clicking on the Generate Areally button opens a new pop-up window. If the Advancing-front mesh generator is selected (Section 4.5), you are asked to enter the desired number of elements for each of the superelements. If you are using TMesh, Triangle or Transport mapping the **Mesh density display/editor** is opened which allows you to set the number of elements for each superelement.

The left part of the window shows the number of elements which will be created for each superelement. The generation is invoked by clicking the **Start** button.

(Re-)Compute element number distribution distributes a given total number of elements (default

1000) on the superelements. To change the number of elements for a particular superelement click on the corresponding superelement number and type the new value in the **Edit number of elements** line. If **Autozooming** is selected, the working window is automatically zoomed to the selected superelement.

Activating **Area sorting** changes the order of mesh generation: Normally the mesh is generated in the same order in which you have drawn the superelements. If the **Area sorting** option is active, the mesh is generated in the order of the superelement area, from the smallest element to the largest one.

The triangulator can occasionally fail for an inappropriate subdivision of superelement edges. In this case, the generator stops and an alert box presents different ways to continue. Your choices are:

- repeat the triangulation for the last superelement,
- start over from the beginning, or
- break the generation process.

Sometimes, a repeated generation for the same subdivision is successful, because the generator dynamically increases the number of iterations and allocates larger working arrays.

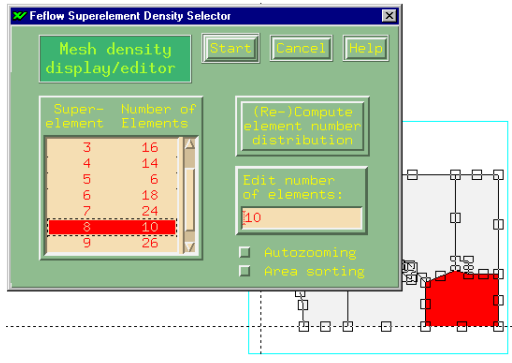
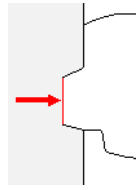


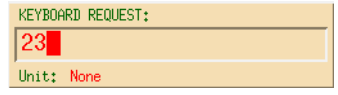
Figure 4.1 Generate areally.

4.4 Generate Gradually



Click on **Generate gradually** to start. This option allows you to input the number of finite elements along each edge of a superelement. The current superelement edge is indicated by an arrow. Note that for edges shared by two superelements the number of elements has to be the same on both sides. Therefore an input is required only once.

This function only works with the **Transport mapping** and **Advancing front** meshing methods as described in Section 4.5.



4.5 Generator Options

The **Generator options** item defines rules for the generation of the finite-element mesh.

FEFLOW implements three different mesh generators:

- **Transport mapping** for quadrilateral elements,
- **Advancing front** for triangular elements at superelement meshes without add-ins and
- **TMesh** (Delaunay) for triangular elements at superelement meshes including add-ins.

Additionally, an interface is provided for the **Triangle** (Delaunay) generator for complex superelement meshes including a large number of add-ins (copyright by J. R. Shewchuk, University of California at Berkeley).

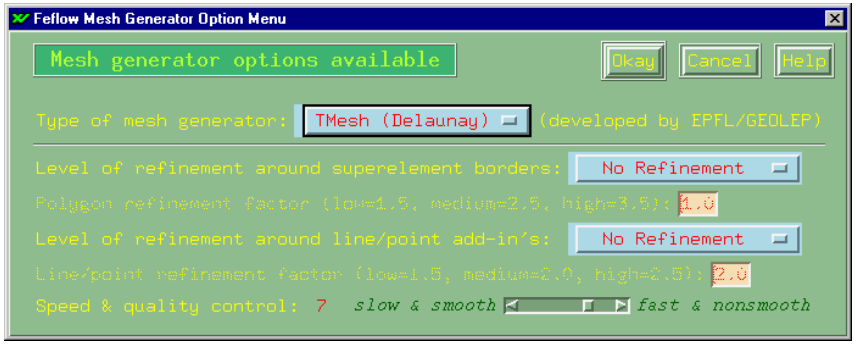


Figure 4.2 Mesh generator options.

Transport mapping/advancing front

Transport mapping creates quadrilateral finite elements while **Advancing front** is a mesh generator for triangular finite elements. Having selected one of these tools the menu displays the options as described below:

- **Iteration number for triangular-mesh smoothing**: Set the value higher if you want a better mesh smoothing, but be aware that it might take much more time, especially if the number of elements is large. Only valid for Advancing front meshing.
- **Triangulation based on quadrilateral supermesh elements**: A triangle mesh will be generated which is similar to a quadrilateral mesh where each quadrilateral element is subdivided into two triangles. With this option you get a very regular distribution of finite elements. Only valid for Advancing front meshing tool and quadrilateral superelements.
- **Automatic zooming during the areal and gradual meshing process**: Automatically zooms to the current supermesh element. The smallest superelement will be shown first.

TMesh (Delaunay)

This generator, developed at the EPFL-GEOLEP Swiss Institute of Technology, Laboratory of Geology, Lausanne, Switzerland, allows to comfortably define the local variation of mesh density.

Having selected the TMesh meshing tool by clicking on the uppermost light blue button the following menu items become visible:

- **Level of refinement around superelement borders**: Specify a refining factor for the finite element mesh along the superelement borders.
- **Level of refinement around line/point add-ins**: If you have designed add-ins (Section 3.5) you can define here how the mesh should be refined along the lines and/or around the points.

***Notice**: Mesh generation by TMesh with medium or high refinement requires significantly more computational effort and accordingly more time for the meshing process.*

Triangle (Delaunay)

The Triangle mesh generator, developed by J. R. Shewchuk, provides a fast triangulation algorithm for triangular meshes including a large number of add-ins. Several options are available to control the meshing process, which can be used individually or combined. Most important are the following options: The **Quality**

Mesh (*q*-switch) option constrains the minimum angle of the triangles. This angle can be directly prescribed. Furthermore, using the *L*-switch option the triangulation can be forced to be a **Delaunay** for all triangles, not just a constrained Delaunay. Commonly, the **divide and conquer** Delaunay meshing algorithm is preferred. Alternatively, the *i*-switch option performs the **incremental** Delaunay meshing algorithm.

4.6 Select Elements

Notice: Unresponsive toggles indicate that the current meshing option does not apply to this element type. To change to an appropriate element type, change the corresponding option in the Shell Options menu (Section 2.6). 6-noded triangles and 15-node prisms are currently not supported.

Before finite-element meshes can be generated, the type of finite elements must be selected.

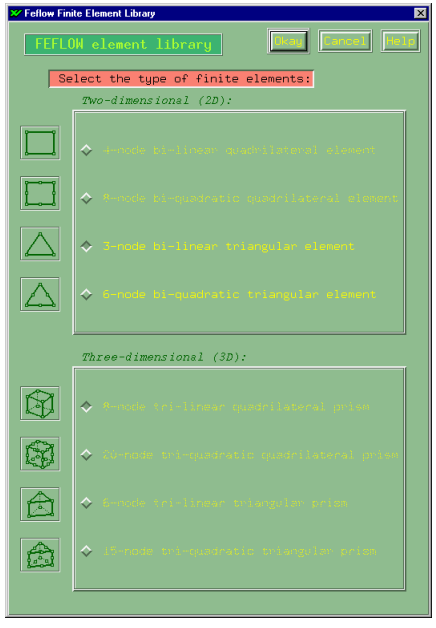


Figure 4.3 FEFLOW element library.

Defaults

Because defaults are available, the novice user may skip this section. Defaults in 2D are the linear 4-nodal quadrilateral element for the mesh quadrangulation option, and the linear 3-nodal triangular element for the mesh triangulation option. In 3D, the corresponding defaults are the 8-nodal quadrilateral prism and the 6-nodal triangular prism, respectively.

Finite element mesh selection

A current element library is shown when the **Select elements** option is chosen. From this library, you may select an element type for the FEM generation. Set the corresponding toggle on the library submenu to specify the element type you choose. Higher order elements (8-nodal quadrilateral and 6-nodal triangle in 2D and 20-nodal prism and 15-node prism in 3D) may lead to a more accurate numerical result for the same number of elements compared with linear element types, at the expense of greater computational effort.

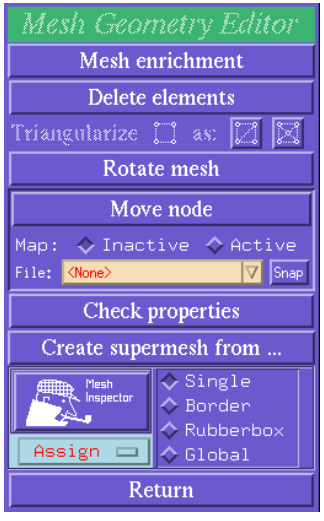
4.7 Continue Mesh Design

This option allows to return to the mesh-design process (described in Section 3) for further superelement design or modification. If a finite-element mesh has already been generated, a warning (alert) box appears to ask you whether the generated mesh should be saved (Save button), or discarded (Abandon button) before entering the mesh editor again. Pushing the Cancel button closes the alert box without further action.

Figure 4.4 Alert box.

4.8 Mesh Geometry

Selecting this item invokes some tools for editing the mesh.



Mesh enrichment

Use the **Mesh enrichment** menu item to locally refine or derefine a finite-element mesh. This can be useful if local mesh refinements or improved mesh accuracy are desired in areas where large gradients are expected.

The enrichment can be executed using the mouse alone or based on polygons or lines using the assigning and joining techniques described in Section 5.6.

Delete elements

The special option **Delete elements** may be useful whenever a mesh contains elements which should be excluded from the computation, for example, areas having a negligible permeability. This approach is often better than assigning extremely small permeability values, which can lead to stiff and ill-conditioned matrix equations that are hard to solve.

***Notice**: Use the deletion with care to avoid 'muti-lated' meshes. Interconnected boundary conditions can also disappear.*

Triangularization of quadrilateral meshes

This tool converts quadrilateral meshes to triangular ones.

As indicated by the buttons you can subdivide one quadrilateral element either into two or four triangles. Splitting into two triangles can be performed using either the shortest diagonal of each element or a consistent splitting direction. Applying the triangularization results in very regularly meshed models.

Rotate mesh

This option allows to rotate a finite-element mesh in the *x*-*y* plane. It is useful to align the domain to a given gravity direction, for instance, with slope laws for

unsaturated or density-driven problems. After setting the center point of the rotation either by mouse click or using the Fixator by hitting <F2>, you are prompted for the rotation angle. An alert box asks you to confirm or discard the rotation.

Move node

Use this option to move a single node of the finite-element mesh. The moving operation is performed either by clicking and dragging a node or by using the Fixator. To invoke the Fixator click the node, keep the left mouse button pressed and hit <F2>.

Node movement is also possible with background maps where the nodes can be snapped to line or point data.

Notice: If moving nodes in a 3D mesh the z-coordinates are automatically interpolated according to the slice elevations of the mesh.

Notice: It is entirely legitimate to create meshes containing interior holes, e.g., where an aquifer crops out.

Check properties

This button opens the Mesh property checker. **Indicate all obtuse triangles** shows all obtuse-angled elements in the mesh (triangles containing an angle greater than 90°), which may cause numerical problems. You should change the supermesh and/or the finite-element mesh to avoid such elements. To achieve a better conformation of the finite-element mesh to the problem and to reduce the number of obtuse-angled elements, choose **Node movement by Laplacian operator on hydraulic head distribution**. In order to detect ill-connected superelements the option **Count number of interior holes** can be helpful. **Measure total area and volume of the domain** allows to calculate the complete area and volume of the model.

Create supermesh from ...

The function 'Create supermesh from outer border geometry' allows saving of the outline of the finite element model as a new superelement mesh.

4.9 Problem Summary

The **Problem summary** gives an overview about the settings of the model. It can be invoked on different levels in the FEFLOW pre- and postprocessing menus.

The following information will be presented:

- File name - specification of the file including data type (ASCII or binary) and version number
- Problem title
- Most **Recent updating** - time of the last data manipulation
- Problem **Dimension** - 2D or 3D problem
- Problem **Type** - saturated or unsaturated
- **Number of layers**
- **Number of slices**
- **Problem measure -** width of the working window
- **Vertical exaggeration**
- **Projection** - horizontal, vertical, or axisymmetric, confined or unconfined aquifer
- **Problem class** - flow and/or transport process
- **Time class** - steady or unsteady flow
- **Time-stepping scheme** - fully implicit or Crank-Nicolson - with constant or varying time-steps - automatic time stepping with different strategies
- **Upwinding** - no upwinding, streamline upwinding, full upwinding, shock capturing or least square upwinding
- **Element type** - 4-, 8-, 3-, or 6-nodal elements in 2D, 8-, 20-, 6-, or 15-nodal prismatic elements in 3D,
- **Mesh elements** - number of generated elements
- **Mesh nodes** - number of generated nodal points

- **Mesh optimization** - indicates if nodal reordering techniques have been performed (required for direct equation solvers)
- Information about **Flow boundaries**, **Flow initials** and **Flow materials** - conditions already set (you can determine whether initial and material conditions have been set or remain at default value, and whether boundary conditions are specified or unspecified.)
- Information about **Transport boundaries**, **Transport initials** and **Transport materials** - conditions already set (as above)
- Completeness of the current problem for running the simulation - **Yes/No**

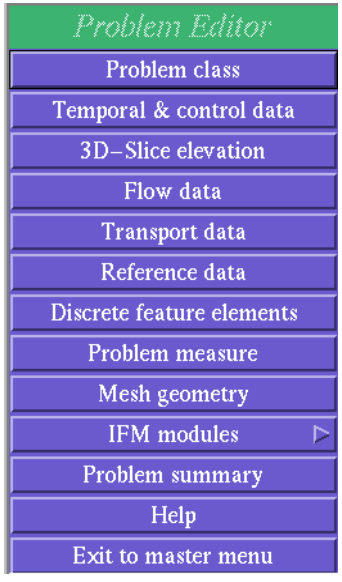
4. Mesh Generator Menu Items

Problem Editor Menu

5

5.1 Introduction

While the **Mesh editor** defines geometric data, the **Problem editor** edits all remaining attribute data such as material properties or initial and boundary conditions. The **Problem editor** also allows the definition of the simulation type and the editing of the simulation-control parameters.



The following main menus are available:

Problem class

Serves for editing the title, general type of problem (saturated or unsaturated media), problem class (steady or transient flow or transport simulation), projection, and the handling of free surfaces.

Temporal & control data

Sets parameters which control the simulation run and offers input tools for time-varying data.

3D-Slice elevation

Configures the vertical extent of the layer and the geometric relations for a 3D aquifer system.

Flow data

Provides submenus for the setting of all parameters defining a subsurface flow problem (Section 5.5). It also gives access to the editing menus for initial, boundary, and material conditions.

Transport data

Offers a submenu structure similar to the **Flow data**

menu for all parameters defining a contaminant mass and/or heat transport problem.

Reference data

Provides submenus to control the settings for comparison of measured and computed values.

IFM modules

Controls which external program modules are used within the current model. Please refer to Section 11 and the online **Help** for detailed information concerning the FEFLOW Programming Interface.

The **Problem measure** (Section 3.8) menu, the **Mesh geometry editor** (Section 4.8) and the **Problem summary** (Section 4.9) were described in the previous sections. In the following subsections, we discuss the main properties of the editor in detail. Note that all working steps within the menus can be carried out with or without zooming.

5.2 Problem Class

The **Problem classifier** dialog has three functions: specifying the problem title, setting the problem class, and specifying the problem projection. Refer to the **Reference manual** for background information on problem classes and projections. The current problem title can be changed to a new project title, which will appear in the data files.

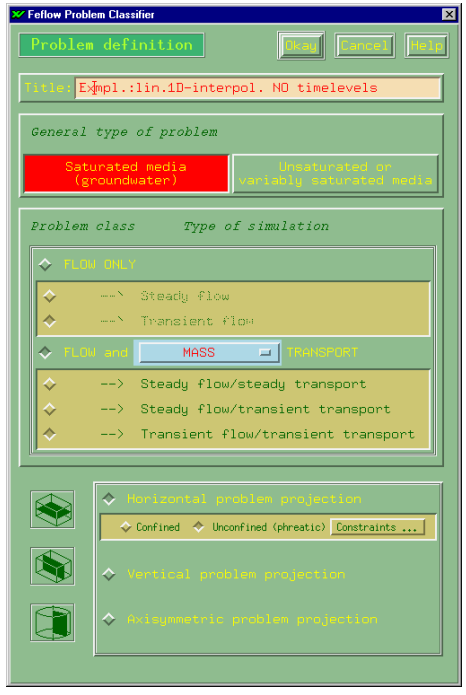


Figure 5.1 Problem definition.

The *General type of problem* distinguishes between the classical **Saturated media (groundwater)** approach and **Unsaturated or variably saturated media**.

A problem can have one of two distinct problem classes:

- **Flow only** or
- **Flow & mass/heat/thermohaline transport**

Types of simulation in the **Flow only** class are steady and transient flows. For unsaturated problems a choice between the standard Richards equation and steady-state linearization has to be made. Steady-state linearization is an extremely fast solution method whose applicability is restricted to special conditions. For further information see online **Help** and the FEFLOW White Paper 'Steade-state linearized Richards equation for fast solution of unsaturated flow systems (FUSY)'.

In the **Flow & transport** problem class, there are three choices:

- steady flow and steady transport,
- steady flow and transient transport (default), or
- transient flow and transient transport.

Please note that in 'steady flow and transient transport' mode only one iteration is performed for the flow. That means that the initial conditions for flow have to reflect steady state conditions!

Also, different cases of 2D problem projection can be selected:

- horizontal (default),
- vertical, or
- axisymmetric problems.

Horizontal problems are aquifer-averaged flow and transport processes, while vertical and axisymmetric problems correspond to cross-sectional and meridional models, respectively. Vertical and axisymmetric projections are the only available 2D projections for unsaturated media and for gravity-affected, fluid density-coupled problems. 2D vertical or axisymmetric models in saturated mode are always confined. To represent free surface conditions an unsaturated simulation has to be performed for such kind of models. Note that for axisymmetric problems the axis of rotation corresponds to the vertical y-axis (where the x-coordinate is zero).

For horizontal problem projection, optional toggle buttons are available to switch between confined and unconfined aquifers. Unconfined aquifers can either have a 'free and movable' top slice or be marked as 'phreatic' where unsaturated flow is computed for dry areas using a simplified approach. Note that an unconfined, free surface aquifer model leads to a nonlinear problem formulation.

For three-dimensional saturated-flow problems with free surfaces, an additional **Free surface definition** menu is available for defining multiple free surfaces and movable slices. For more detailed information please see the FEFLOW online **Help** and the Tutorial (Section 10.3.2.1).

The model can be transformed from a transient to a steady-state model by changing the **Type of simulation** in the Problem Class menu**.** If time-dependent boundaries, constraints or flow material exist, a special window appears where you can insert the steady-state time step. The boundaries and parameters are interpolated and then set constant.

5.3 Temporal & Control Data Menu

Essential parameters that control the stability and accuracy of the simulation are defined here. The parameters include: number of time steps, type of time stepping, final time, level to switch to Crank-Nicholson (CN) higher-order scheme, error tolerance and convergence criteria, types of upwinding, and nature of the time-varying functions.

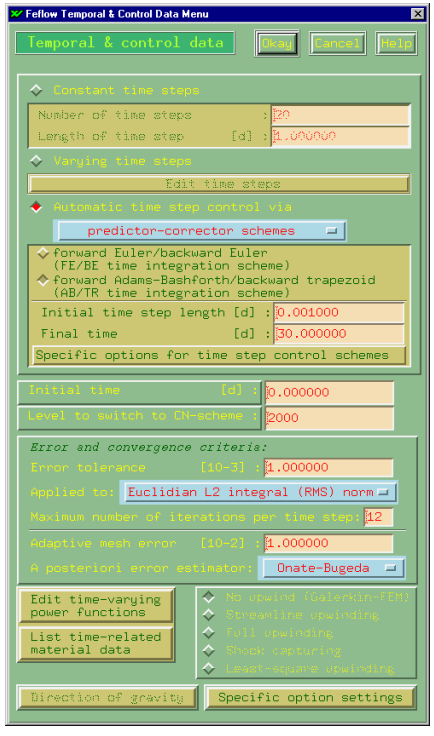

Fellow Temporal & Control Data Menu
Temporal & control data
Okay
Cancel
Help
Constant time steps
Number of time steps : 20
Length of time step [d] : 1.000000
Varying time steps
Edit time steps
Automatic time step control via
predictor-corrector schemes
forward Euler/backward Euler (FE/BE time integration scheme)
forward Adams-Bashforth/backward trapezoid (AB/TR time integration scheme)
Initial time step length [d] : 0.001000
Final time [d] : 30.000000
Specific options for time step control schemes
Initial time [d] : 0.000000
Level to switch to CN-scheme : 2000
Error and convergence criteria:
Error tolerance [10-3] : 1.000000
Applied to: Euclidian L2 integral (RMS) norm
Maximum number of iterations per time step: 12
Adaptive mesh error [10-2] : 1.000000
A posteriori error estimator: Onate-Bugeda
Edit time-varying power functions
List time-related material data
No upwind (Galerkin-FEM)
Streamline upwinding
full upwinding
Shock capturing
Least-square upwinding
Direction of gravity
Specific option settings

Figure 5.2 Temporal & control data.

Time steps

Transient simulations require temporal discretization. You can choose between **Constant time steps**, **Varying time steps**, and **Automatic time step control**. This last choice also allows to you select between different adaptive schemes. For constant time steps, the default setting is 1 day. Note that time steps are not applicable for steady-state problems.

Constant time steps usually reduce the numerical effort during the simulation because the simulator can use efficient resolution techniques. This avoids updating the matrix system for linear problems in a time-step marching process.

Varying time steps can be entered directly in a **Time-step editor**, or may be imported from a database.

The **Automatic time-step control** can be performed using either the **Forward Euler/backward Euler (FE/BE)** time-integration scheme, which is 1st order in time (often appropriate for density-driven and unsaturated problems), or the **Forward Adams-Bashforth/backward trapezoid (AB/TR)** time-integration scheme, which is 2nd order in time. For variably saturated problems the **Aggressive target-based time-marching scheme**, either fully implicit or semi-implicit, may provide an effective solution strategy.

Pushing the button **Specific options for time step control schemes,** constraints and specific options for the automatic time-stepping process can be set.

Level to switch to CN-scheme

Sets the level to switch to Crank-Nicolson (CN) higher-order scheme (not applicable to automatic time-step control). The default is 2000. This means that up to the 2000th time step, a standard, fully implicit time-stepping scheme with first-order accuracy is used. Subsequently, the second-order accurate CN scheme is

employed. While the implicit scheme is unconditionally stable, the CN-scheme can cause oscillations. Set the level to zero to use the CN-scheme from the beginning.

Error and convergence criteria

The **Error tolerance** controls termination of the iterative procedure for both nonlinear density-coupled flow and transport, nonlinear processes in unconfined aquifers and nonlinear flows for unsaturated media. Note that the error is dimensionless. Its default value is 0.001. The parameter has no meaning for linear (e.g., horizontal and/or confined) problems. Setting a smaller values enforces higher accuracy and implies increased numerical effort, i.e., more iterations before termination. The error norms are defined as follows:

The **Euclidean L^2 integral root mean square (RMS)** error norm is the default error norm to measure an integral error quantity. The **Absolute L^1 integral** error norm represents an average of absolute deviations of the error in the solution domain. The **Maximum L_∞** error norm can be useful to focus on the maximum error occurring in the solution. It is the strongest measure and should be used if the local error is important in the numerical process ('scheme listens to each sound').

Modify the setting of the **Maximal number of iterations per time step** for problems which need many iterations to meet the convergence criterion. If the error does not fall below the criterion during the given number of iterations an error message is produced in the Log window.

Adaptive mesh error and the ***A posteriori* error estimator** define the computation of the **Adaptive mesh refinement** (See Section 2.6).

Refer to the White Paper 'Error norms used in FEFLOW' (Chapter 5 of the White Papers Vol. I) for additional information.

Upwinding

Five types of **Upwinding settings** are available to stabilize numerical results for mass and heat transport problems:

No upwinding (Galerkin-FEM approach) This is the default option and produces the best accuracy; however, it may lead to oscillations in the concentration or temperature results if convection-dominated transport processes are modelled on coarse meshes.

Streamline upwinding is recommended if oscillating results have been produced. It stabilizes the computation by introducing a streamlined damping measure (numerical dispersion).

Full upwinding remains the last resort for damping oscillations, if all other types have failed. However, it can generate a great amount of numerical dispersion.

Shock capturing adds a nonlinear anisotropic damping factor to stabilize convection-dominant transport processes. This powerful method removes numerical oscillations at abrupt changes or fronts of the solution with a minimal amount of numerical dispersion. It is only available for adaptive time-stepping schemes.

Least-square upwinding represents an alternative numerical scheme to solve transient advection-dispersion transport problems. In contrast to standard techniques it leads to symmetric matrix systems and possesses a built-in streamline-like upwind characteristics.

***Notice**: For further information refer to the FEFLOW White Paper 'The Petrov-Galerkin least square method (PGLS)'.*

Direction of gravity

Use this option to change the direction of the gravity vector for the model.

Specific option settings

Offers access to special numeric settings. You can enter the same menu from the shell **Options** menu (see Section 2.6).

5.3.1 Edit time-varying power functions

Invokes the **Power function editor**, in which you can edit time-related functions interactively.

An unlimited number of power functions can be created, edited, imported, and exported. The edited power function is displayed automatically as a time-value plot. Power functions are used for time-varying functions such as varying time-steps (this chapter), time-varying boundary conditions or material parameters. Each power function is identified by an integer ID. These IDs are listed in the **Flow data** menus and can be assigned directly or interpolated on the mesh as boundary conditions, constraints or material parameters. To each function you can add a comment, e.g., the name of an associated well.

There are different types for the curves:

- Polyline: the value pairs (time/function values) are connected by linear interpolation.

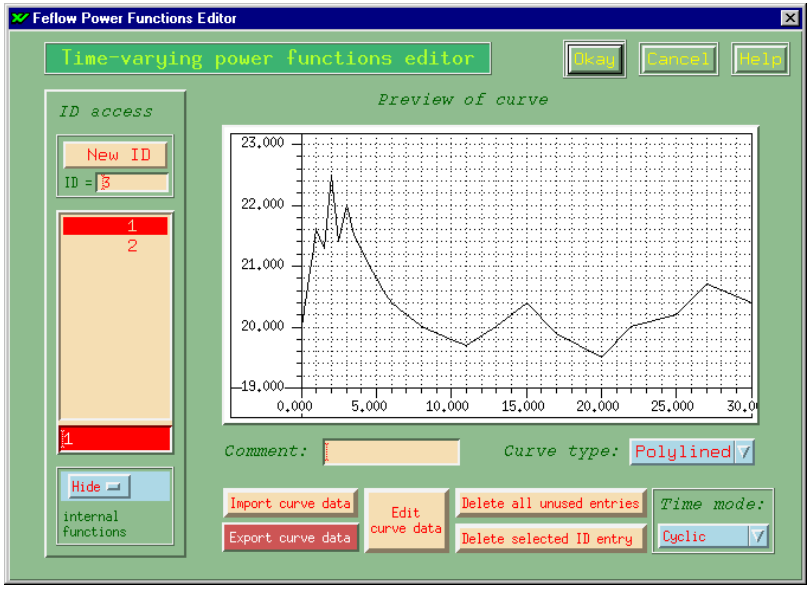


Figure 5.3 Time-varying power functions editor.

- Constant: the function values define a stepwise constant function. For the ramp steepness an internal value of 89.994° is used.
- Akima uses a third-order polygonal smoothing based on the given values.
- Akima2 smooths the function using additional middle nodes.

Each function can be applied in one of two time modes:

- non-cyclic
- cyclic

In non-cyclic mode the function value is held constant after the simulation time has reached the last time value defined in the time-varying function. In cyclic mode the function is applied again from its beginning and until the simulation ends. Use this mode to apply, for example, annual hydrographs in a multi-year simulation.

5.3.2 List time-related material data

In FEFLOW all material data can vary over space and time. The data are assigned via the **T-List** tool or the **Join tool** in the **Material data** menus of the **Flow data** and **Transport data** options (Section 5.5 and Section 5.9).

The submenu termed **Material data time list menu** displays, for each material parameter, the time values for which material distributions are defined. During the simulation, the current value is obtained by interpolating between these given time steps, either linearly (‘Polylined’) or using a third-order polygonal smoothing (‘Akima’).

Time-related material data can be applied in linear (non-cyclic) or cyclic mode (see Section 5.3.1).

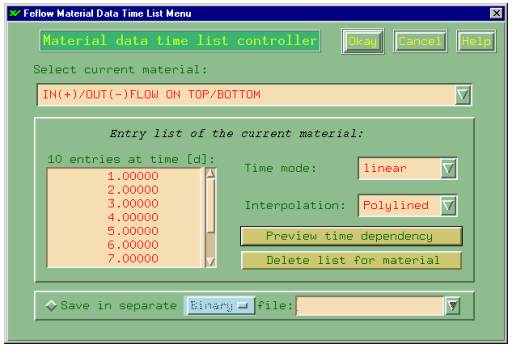


Figure 5.4 Material data time list controller.

Time-related material data is stored either in the problem file (*.fem) or in an external ASCII or binary file (*.mli). Specify the name of the external file in the input field.

The **Preview time dependency** button opens a plot window for the time-varying data for each element in a diagram.

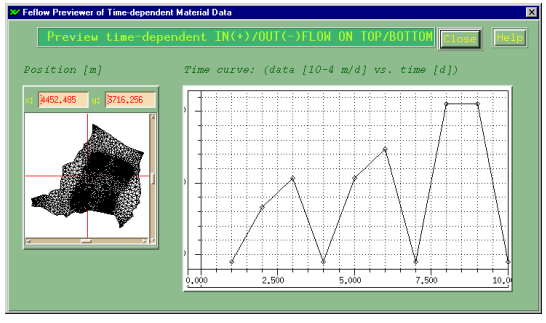


Figure 5.5 Preview time dependency of material data.

To delete the entire material list push the **Delete list for material** button.

5.4 3D Slice Elevation

This submenu allows you to define, control, and plot the elevations of the single slices in a 3D problem.

Use the ***z*-coordinates** button to assign the elevations to the nodes. Besides the 'Global' and 'Nodal' mode a linear interpolation method ('Skew plane') and different regionalization methods for imported data ('Database') are available.

Click **Reconfigure 3D task** to enter the Layer configurator window. The Layer configurator allows you to visualize and modify the different layers and slices and their elevations in a 3D model (see Section 10.4.2).

To avoid intersection of slices during the assigning of z-elevations a minimal slice distance can be defined in the **Slice distance modifier**.

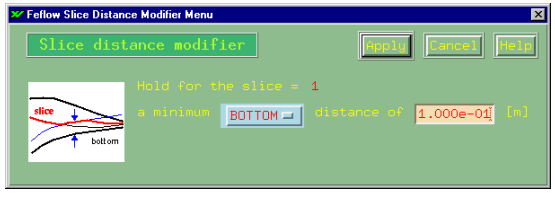


Figure 5.6 Slice distance modifier.

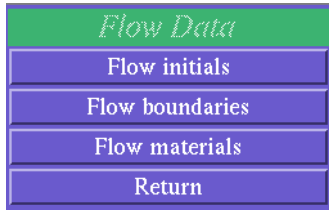
For more detailed explanations see FEFLOW online **Help**.

5.5 Flow Data

Initial conditions, boundary conditions, and flow material parameters can be displayed and edited.

Pushing the **Flow data** button in the Problem Editor menu invokes the **Flow data** submenu.

The first item, **Flow initials**, opens a submenu for assigning and viewing the initial hydraulic head conditions. More information about this item is available in Section 5.6.



The **Flow boundaries** option enables you to edit first-, second-, third-, and fourth-type boundary conditions and constraints in a separate submenu. Parameter values can be entered either graphically using the 'Nodal', 'Border' and 'Rubberbox' options or by different 1D and 2D 'Database' interpolation methods. Both stationary and time-varying boundary conditions can be assigned. The definition of constraints for the boundary conditions is executed via submenus.

The **Flow materials** option displays a submenu for editing all material parameters necessary to desribe a saturated or unsaturated flow problem. Parameter values can be set globally or locally. Local stationary or time-varying values can be assigned elementwise, by using a template, by kriging and Akima interpolation, or by extrapolation from databases.

5.6 Flow Initials

When **Flow initials** is selected from the **Flow data**

menu, a submenu appears to specify initial conditions for flow. The following interactive, mouse-supported tools are available to enter, edit, and plot flow initials:

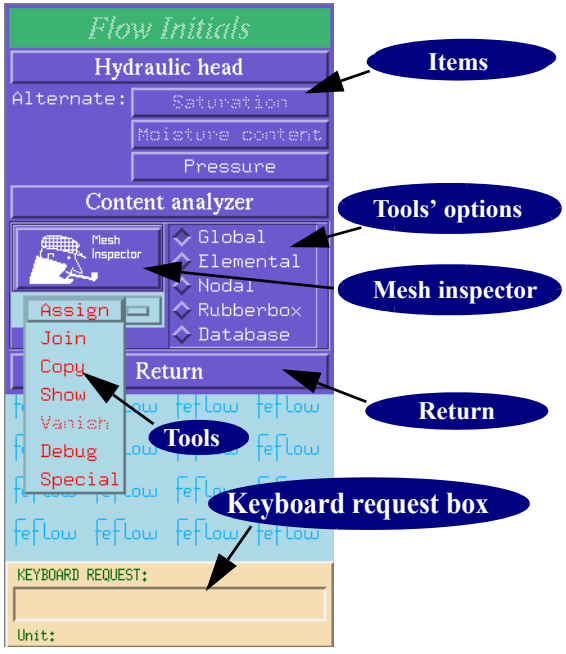


Figure 5.7 Flow Initials submenu.

Assign

Manages the keyboard-controlled and mouse-based input of data and regionalization from databases. Choose from the following input types:

- **Global** - Uniform value for the whole model (2D) or the current slice (3D),
- **Nodal** - Specific value for mouse-selected single nodes,
- **Elemental** - Specific value for mouse-selected single elements,
- **Rubberbox** - Uniform value for an area marked by a rubber box,
- **Database** - Values from a database by regionalization (Figure 5.8). The databases can be ESRI Shape files, dBASE files or ASCII databases. Using ASCII databases you have to select the appropriate columns for the (x, y)-coordinates and for the function value, or the data have to be prepared as so-called triplet files using the format: ***x-coord. y-coord. function-value***.

In the Flow initials menu you can regionalize stationary data only, where the function value describes the constant value. In the Flow boundaries and Flow materials menus transient data can be regionalized, too. For examples please refer to the Demonstration Exercise book and the Tutorial (Section 10), or invoke the FEFLOW online **Help** hitting <F1>.

Copy

Is mostly used for 3D problems. It copies flow initial data from the current slice to other slices. Do not forget to assign flow initials to each slice, not just the top one! The Advanced option allows copying of an initial distribution to a reference distribution with a given identifier. Reference distributions can be used as a placeholder for data (see Section 5.10). For a detailed description of the different options see the online **Help**.

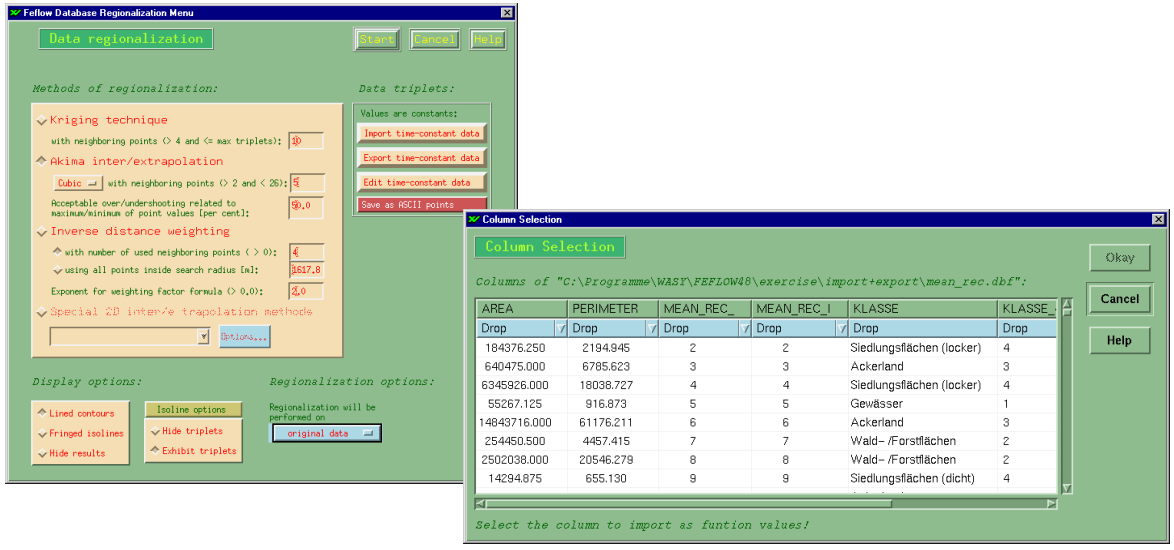


Figure 5.8 Database regionalization window and column Selection.

Join

Allows you to use ASCII or Shape file polygons, or FEFLOW supermeshes, as templates. You can interactively set values for each subarea, interpolate triplet files on selected subareas or import a value for each subarea automatically by linking the ID of the subarea with a column of an Arc/Info, ASCII or a dBase database. It is also possible to assign values from a database to different timesteps of time-varying material data (see Section 10.3.4.3).

The linking of a polygon file with a database is supported by a submenu.

See the online **Help** for detailed information and have a look at the application example of the FEFLOW Tutorial (Section 10.3.2.2).

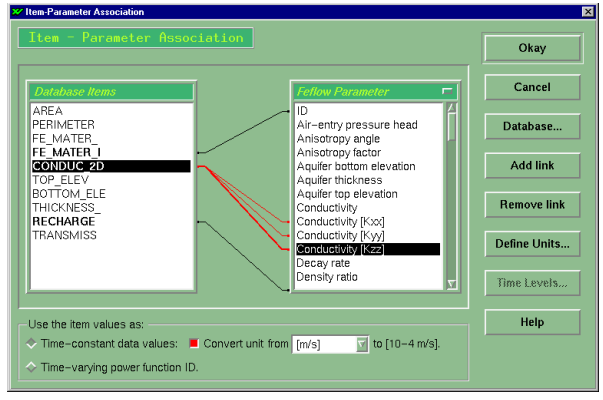


Figure 5.9 Linking of database with spatial data file.

Debug

Displays and modifies data groups. Data ranges or subareas of the model domain (via background maps) can be selected and the corresponding values can be changed by adding/subtracting, multiplying/dividing, or simple replacing operations.

Show

Plots the flow initials as colored fringes (Figure 5.10).

Vanish

Switches off the Show option.

Special

Allows data visualization and export via the **Data store manager** (**DSM**), which is available from other menus, too. The **DSM** manages the import and export of spatial data in predefined or user-defined file formats that can be linked with attribute data. See online **Help** for more information. The **Special** menu also allows to compute 'Head minus bottom' and 'Top minus Head' isoline-maps.

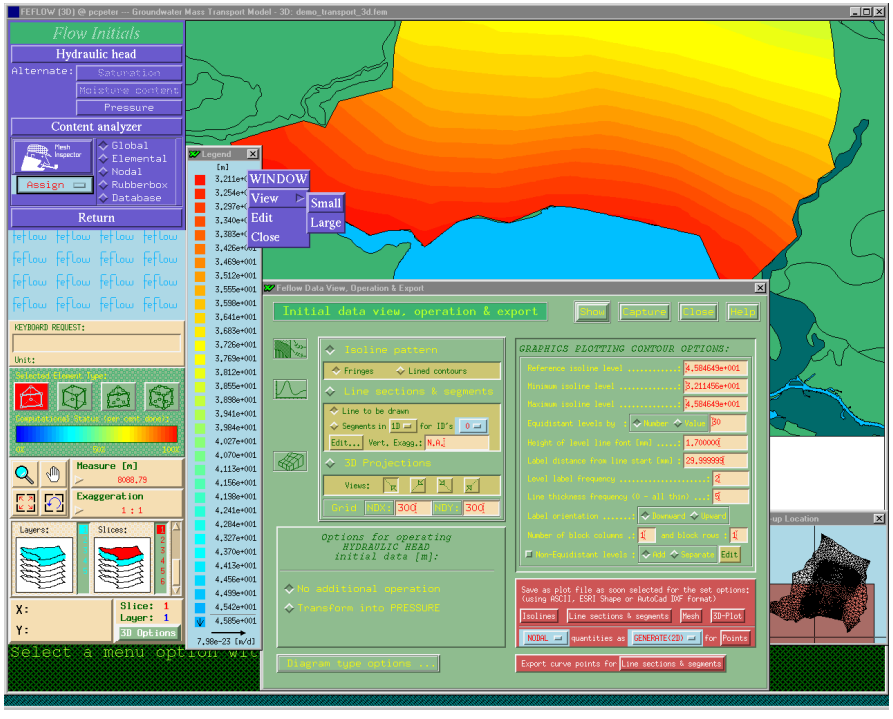


Figure 5.10 Special menu.

Mesh Inspector

Displays the current value and physical units for the node in the **Inspector** magnifier. If an ESRI shape file has been loaded, its attribute values are listed in a second **Database inspector** window (Figure 5.11).

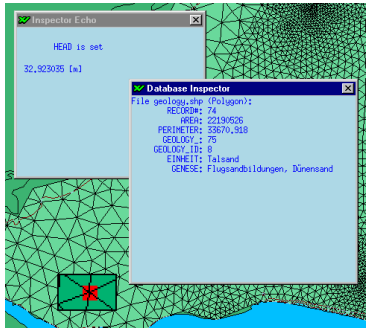


Figure 5.11 Mesh Inspector echo.

Keyboard request box

Accepts keyboard input. Having selected an option of a tool which requires keyboard input a default entry is shown here. To change the value click into the box, select the default value with the mouse in order to replace it or hit the <TAB> key. Below the box the physical unit of the input value is displayed.

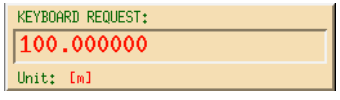


Figure 5.12 Keyboard request box.

Return

Click this button to return to the upper menu level.

Content analyzer

Offers functionality for computing the fluid/mass/energy content of the model. There are eight different contents to evaluate. They are listed in Table 5.1.

Table 5.1 Content analyzer options

$\int dV$	Total volume [m³]
$\int \varepsilon dV$	Void volume [m³]
$\int s\varepsilon dV$	Fluid content [m³]
$\int s\varepsilon C\, dV$	Diluted mass (fluid phase) [g]
$\int s\,(1-\varepsilon)\,\chi(C)\,C dV$	Sorbed mass (solid phase) [g]
$\int s\varepsilon\rho^f c^f T dV$	Energy of fluid phase [J]
$\int (1-\varepsilon)\,\rho^s c^s T dV$	Energy of solid phase [J]
$\int \left[s\varepsilon\rho^f c^f + (1-\varepsilon)\,\rho^s c^s\right] T dV$	Total energy content [J]

The content analyzer is provided in all three (flow, mass and heat transport) initial-value menus as well as in the simulator and the postprocessor menus.

5.7 Flow Boundaries

The **Flow boundaries** menu supports the input of the boundary conditions for the flow equations. Boundary conditions can be stationary or time-varying. All

boundary conditions can be limited by *Constraints*. A detailed description of the different types of boundary conditions is given in the Reference Manual. The boundary conditions are:

- **Head** (first type, Dirichlet, [m]): It describes a fixed potential at a node.
- **Flux** (second type, Neumann, [m/d], [m²/d]): Assigns a flux to a node, for a 2D horizontal confined model the flux is considered depth-integrated. The boundary condition is only valid if you define a distance over which it should apply by selecting adjacent nodes.
- **Transfer** (reference hydraulic head, third type, Cauchy, [m]): Defines a reference hydraulic head of a domain outside the model such as a river or a lake. The boundary condition is only valid if you define a segment along which it should apply by selecting adjacent nodes. You have to define a *Transfer rate* in the **Flow materials** menu (Section 5.8) for the leakage arising between this reference hydraulic head and the aquifer.
- **Well** (fourth type, [m^3/d]): Describes the injection or withdrawal of water at a single node.

It is possible to constrain the boundary conditions by setting *Constraints*. The **Constraint conditions of Flow boundaries** submenu is opened by clicking the arrow to the right of each boundary condition button.

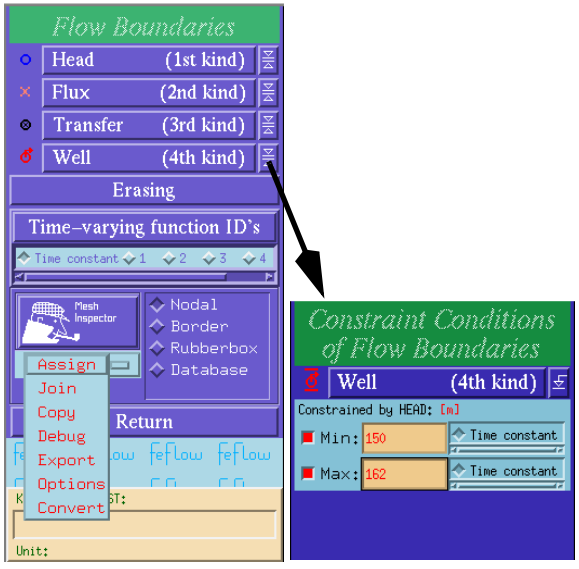


Figure 5.13 Boundary and constraint conditions menus.

You can limit a potential boundary condition by maximum and minimum bounds for flux, or a flux boundary condition by maximum and minimum values for the resulting hydraulic head. Transfer boundary conditions can be limited either by head or by flux, while well boundaries are constrained by head. Furthermore, all constraints can be edited as time-varying functions.

For a better understanding of these options please refer to the Demonstration Exercise and the Tutorial section.

Boundary and constraint conditions will be displayed as symbols on the nodes and can be checked by using the **Mesh inspector**. A second window, the **Database inspector** displays the properties of the background map, if present (ESRI shape file).

We recommend to read the corresponding section in

***Notice**: For further information about the head constraint for 3rd-kind boundary conditions refer to the White Paper 'Extended formulations of constraints for Cauchy-type (3rd kind) boundary conditions in FEFLOW'.*

***Notice**: Outfluxes are defined as positive for boundary conditions. However, for constraint conditions the definition is opposite, here influxes are positive!*

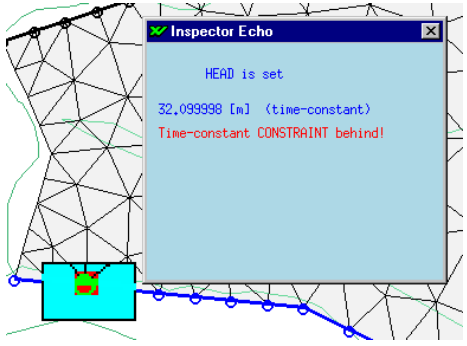


Figure 5.14 Mesh inspector.

the Reference Manual and to use the online **Help**.

In addition to the standard commands of the **Flow data** menus, the **Flow boundaries** menu offers the following tools and functions:

Erasing

Deletes some or all of the boundary conditions via a cascade pop-up menu. First-, second-, third-, or fourth-type, or all boundary conditions can be erased from the current slice. Use the right mouse button to confirm and execute. Note that a value-related erasing can be performed using the Debug tool (see Section 5.6).

Time-varying function IDs

Controls assigning of time-varying boundary conditions by assigning power functions. Click on **Time-varying function IDs** for opening the **Power Functions editor** (which you can also enter from the **Temporal & control data** menu, Section 5.3.1). A slider bar below the button contains the ID numbers of the currently defined time functions. For any ID shown, the respective toggle can be set to assign the respective function to a time-varying boundary condition.

The left-most toggle (default setting) corresponds to time-constant boundary conditions. Before assigning boundary conditions, you should set the corresponding ID toggle. For time-varying functions, the symbol of the boundary conditions is shown together with the corresponding ID number while stationary boundary conditions are indicated by symbols without an ID number.

Assign

Is similar to the **Assign** tool in the *Flow Initials* menu (Section 5.6), with one additional option: **Border** is a mouse-controlled input of boundary conditions along the boundaries of the model. A constant value can be set, or, by setting a start and an end value, a linear interpolation along the boundary is performed. The **Database** option supports here also the 2D regionalization of time-varying boundary conditions and the direct assignment of database values on the nodes. The latter option is useful to import boundary conditions exported from another FEFLOW model using a similar mesh. For time-varying interpolation the triplet files must contain the ID of a Power function as function values (format of a triplet file: *x*-coordinate *y*-coordinate function-value). See the FEFLOW online **Help** for detailed instructions.

Join

In addition to the basis functionality described in Section 5.6, the **Join** tool supports the 1D regionalization of stationary and time-varying data along lines, for example, for modeling river systems as boundary conditions, and 2D regionalization of time-varying data.

The joining can either be performed interactively or automatically for all lines. The line order for joining can be selected based on the order in the line file or based on the order of an arbitrary database column.

Export

Exports the boundary conditions as ASCII files.

Options

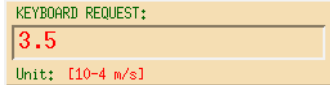
Are only important for flux and transfer boundary conditions in a certain context. Values of flux and transfer can be treated as area-independent, which means that the discharge varies with the cross-sectional area of the effective aquifer, or treated as depth-integrated where a varying cross-sectional area does not affect the quantity of the discharge. For unsaturated flow the flux boundary condition can differ between flux-type and gradient-type conditions. The latter is useful to formulate free drainage boundary conditions.

Convert

Changes type and attributes of boundary conditions, for example, you can convert flux boundaries to transfer boundaries. Note that the values remain constant but the units change.

5.8 Flow Materials

The submenu items explained in this section are used to enter the material conditions for the flow equations. The specific material requirements depend on the problem dimensionality and projection type for 2D problems (horizontal, vertical, axisymmetric) as selected in the *Problem class* menu. Note that these items imply different meanings for the **Tools** button, which can be set either to *Assign*, *Join*, *Copy*, *Show*, *Vanish, Debug*, *T-List, Special or Options*. The **Assign** tool is the default. It allows the assignment of material-parameter values necessary for describing the selected problem type. For more detailed information about these tools see Section 5.6.



The required physical units of each material parameter are indicated in the **Keyboard request** box. The input follows the same steps as outlined above for initial conditions.

In addition to the standard Flow data tools described in Section 5.6, the following tools are available:

Assign

Time-dependent material data can be regionalized using the 'Database' option either from power functions at specified locations or from a database containing the values for each time step in a column. See online help for a detailed description.

T-List

Controls the creation of time-varying material distributions. The **Assign current distribution** option assigns the current material distribution to a time entry, **Copy list data** copies time varying data between layers

and different parameters. **Preview time dependency** plots a diagram for each element. This can also be done in the **Temporal & control data** menu (Section 5.3).

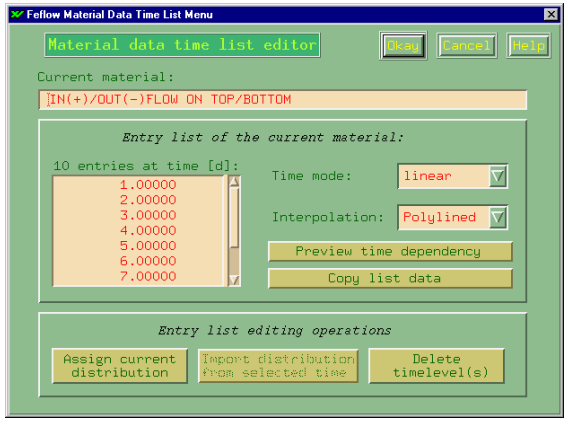


Figure 5.15 Material data time list editor.

Options

Define here if the anisotropy of the conductivity should be oriented to Cartesian coordinate system or to the layer inclination.

Copy

Copy time-varying material-parameter values between layers or to another material parameter (*Advanced* option).

Unsaturated properties

The item **Unsaturated properties** switches to the input menu for unsaturated-flow material parameters. Use this menu to choose between **Van Genuchten**, **Brooks-Corey**, **VG modified**, **Haverkamp**, **Exponential** and **Linear** parametric relationships and to assign the corresponding parameters.

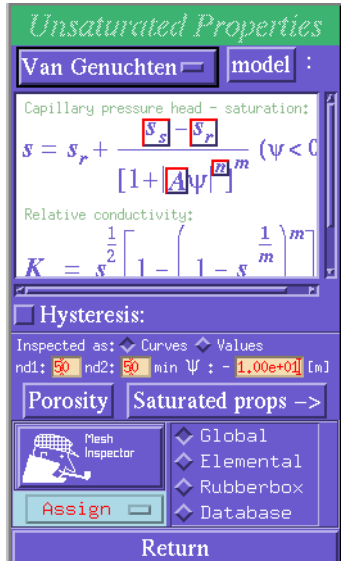


Figure 5.16 Unsaturated properties.

The default setting for the whole model domain is the Van Genuchten relationship. To change the parametric relationship for parts or all of the model, set the switch to the new relation, choose one of the input tools, e.g., assign or join, and click the **model** button. It is possible to use different parametric relations for different areas within one model.

Use the **Porosity** button to assign matrix porosity for unsaturated conditions.

The white box displays the equations corresponding to the active parametric relationship. The parameters to be assigned are enclosed in red boxes. To set a parameter choose any input tool and click the symbol of the parameter in the equation.

Set the

button to incorporate capil-

lary hysteresis in a simulation. Use the switch to change between the wetting curve and the drying curve.

The **Inspected as** line specifies the behavior of the mesh inspector. Choose between viewing saturation vs. capillary head and saturation vs. conductivity **Curves** or the **Values** in text mode. ***nd1*** and ***nd2*** determine the resolution of the curves while **min** ψ prescribes the minimum capillary head for the curve.

Click the **Saturated properties** button to return to the Flow Materials menu.

See the FEFLOW online **Help** for additional information.

In the following Table 5.2 all parameters for saturated and unsaturated flow are listed.

Table 5.2 Flow materials

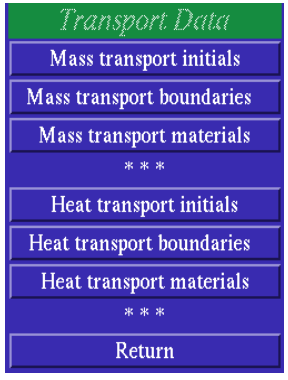
Parameter	Description	Application
SATURATED MEDIA		
Conductivity	Proportional to flow resistance in an aquifer	Major principal direction
Transmissivity	Proportional to flow resistance and aquifer thickness	2D horizontal, confined
Anisotropy factor	Ratio of maximum directional value to its original value	2D
Anisotropy angle	Angle between cartesian x-axis and major direction of anisotropy	2D
Aquifer bottom elevation	Bottom elevation for elements	2D horizontal
Aquifer top elevation	Top elevation for elements	2D horizontal
Storativity	Drain/fillable void space in aquifer	Unconfined aquifer
Density ratio	Mass buoyant expansion coefficient for density coupled flow	2D vertical and 3D modeling
Expansion coefficient	Heat buoyant expansion coefficient for density coupled flow	2D vertical and 3D modeling
Storage compressibility	Tendency of void space to be reduced under pressure	
In-/outflow on top/bottom	Spatially variable recharge/evaporation on top or bottom slice	3D
Source/Sink	Spatially variable recharge/evaporation	2D
Transfer rate in/out	Value computed from conductivity and thickness of colmation layer (“leakage coefficient”)	Required for Transfer boundary conditions

Table 5.2 Flow materials (continued)

Parameter	Description	Application
UNSATURATED MEDIA		
S_s	Maximum saturation	
S_r	Residual saturation	
Ψ_a	Air entry pressure	
Porosity	Total porosity	
$n, A, B, \alpha, \beta, \delta$	Fitting parameters for the different parametric models below	
Van Genuchten	Parametric model for unsaturated flow	
Brooks-Corey	Parametric model for unsaturated flow	
Van Genuchten (VG) modified	Parametric model for unsaturated flow	
Haverkamp	Parametric model for unsaturated flow	
Exponential	Parametric model for unsaturated flow	
Linear	Parametric model for unsaturated flow	

5.9 Transport Data

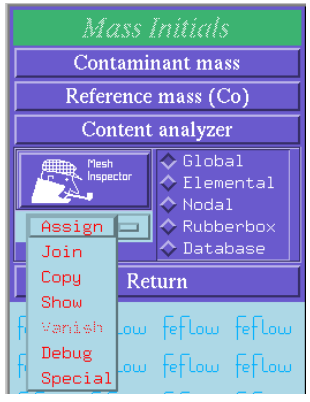
In this section, *initial conditions*, *boundary conditions*, and *transport material properties* for both contaminant mass and heat are specified. Due to the similarity between the parameters for contaminant mass transport and for heat transport, only the contaminant mass transport menus will be described explicitly. For detailed information about the principles and basic equations of transport modeling please refer to the Reference Manual.



Many of the procedures are the same as those in Section 5.5, which is referred to frequently in this section. The **Transport initials** menu offers not only the setting of an initial distribution of the mass concentration but also the possibility to define a reference contamination mass/temperature, which is used for the calculation of the fluid density. For detailed information refer to the FEFLOW online **Help** (hit <F1> in the Transport initials menu) or the Reference Manual The **Transport boundaries** menu is similar to the **Flow boundaries** (Section 5.7) menu. For the definition of the mass boundaries we again refer to the Reference Manual. The **Transport materials** menu differs in the parameters from the **Flow materials** menu. The tables in the Reference Manual give the default units for the transport parameters, and the online **Help** gives more detailed information. You can assign, edit, and debug transport initials, transport boundaries and transport materials. The **Mass transport materials** menu allows you to set the following parameters: **Aquifer thickness**, **Porosity**, **Sorption laws** (Henry, Freundlich, Langmuir) and Coefficients, **Molecular diffusion**, **Longitudinal dispersivity**, **Transverse dispersivity**, **Dispersion type** (Linear, Nonlinear), **Decay types** (First Order, Michaelis-Menten, Decay Chains) and **Rate coefficients** of reaction kinetics, **Transfer rate**, and **Source/sink** of contaminants.

The **Heat transport** data menus are similar to the **Mass transport** data menus. For an explanation of the parameters, see the Reference Manual.

5.9.1 Transport initials



The initial mass concentration (temperature) can be entered globally, element-wise, or node-wise. **Reference mass** concentration and/or **Reference temperature** can be defined for to take into account the influence of viscosity and density on the effective permeability. See Section 5.6 for an overview of how data can be viewed, assigned, and edited. You can also find a description of the Content Analyzer there. For detailed information see the online **Help**.

5.9.2 Transport boundaries

Notice: The conceptual design is similar for all Flow and Transport Data menus. Refer to the Flow Initial Data section for getting an overview of the main functions of these menus.

Notice: The meaning of fluxes' depends on the selection between Convective form transport (default) and Divergence form transport in the Options menu of the Shell. For the former, fluxes are dispersive, i.e., they are controlled only by the concentration gradient. For the divergence form, the total fluxes consist of the convective and dispersive parts. Refer to the White Paper 'About the difference between the convective form and the divergence form of the transport equation' for details.

See Section 5.7 for details on this type of menu (and associated submenus). The following types of boundary conditions may be specified for the transport equations.

- **Mass** (1st kind, Dirichlet), for heat: **Temperature**, known contaminant concentration (or temperature)
- **Flux** (2nd kind, Neumann), for heat: **Heat Flux**, inflow or outflow density of contaminant mass quantity (or thermal energy).
- **Transfer** (3rd kind, Cauchy), inflow or outflow density through a leaching layer, e.g., from a salt dome into overlying aquifer through gypsum layer.
- **Well** (4th kind), single source or sink for contaminant (or thermal energy).

All boundary conditions can be stationary or time-varying. Complementary constraints and constraints for hydraulic head are available for all kinds of boundary conditions. For detailed information about the physical background see the Reference Manual (Section 4.2).

5.9.3 Transport material data

See Section 5.8 for details on this type of menu. Here, the necessary transport parameters are entered and important settings for the computation of mass transport are made. Different sorption isotherms (Henry, Langmuir and Freundlich), two dispersion laws (linear/nonlinear) and three different types of decay (First-order/Michaelis-Menten/Decay chain) are provided for selection. Further information is available in the FEFLOW online **Help.** For a detailed description of the treatment of chemical reactions in FEFLOW refer to the White Paper 'Chemical reactions'.

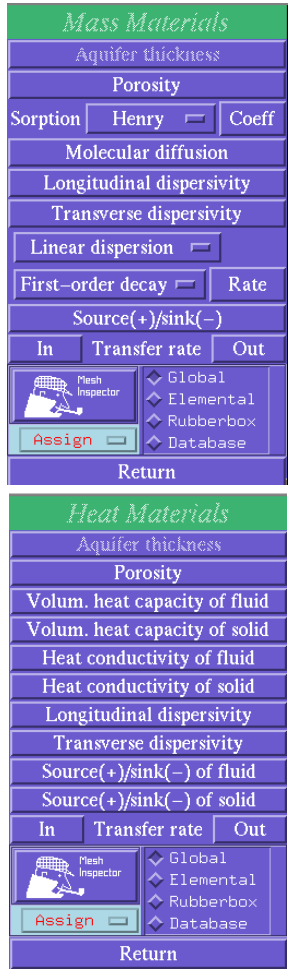


Table 5.3 Mass materials

Parameter	Description
Aquifer thickness	For 2D horizontal, confined aquifer
Porosity	Void space
Sorption coefficient	Sorbed materials described by Henry, Langmuir and Freundlich isotherms
Molecular diffusion	Diffusion of a chemical in solution
Longitudinal dispersivity	Spreading of a chemical due to heterogeneity of the porous medium in flow direction
Transverse dispersivity	Spreading of a chemical due to heterogeneity of the porous medium in the direction orthogonal to the flow
Dispersion parameter beta	Parameter for nonlinear (non-Fickian) dispersion law
Decay rate	Rate of contaminant decay due to biodegradation or radioactivity
Source/Sink	Spatially varying in-/outflux of contaminant mass
Transfer rate	Transition resistance for contaminant mass flux

Table 5.4 Heat materials

Parameter	Description
Aquifer thickness	For 2D horizontal, confined aquifer
Porosity	Void space
Volumetric heat capacity of solid	Heat capacity times density of solid
Heat conductivity of solid	Fourier's heat conductivity coefficient of the solid
Longitudinal dispersivity	Thermo-dispersivity in longitudinal flow direction
Transverse dispersivity	Thermo-dispersivity orthogonal to the flow direction
Source(+)/Sink(-) of fluid	Thermal supply of fluid
Source(+)/Sink(-) of solid	Thermal supply of solid
Transfer rate	Transition resistance for heat flux

5.10 Reference Data

You can insert and edit reference data, such as observation points, grouped balance points, sections or fence segments and nodal distributions for the evaluation of the simulated results. The menu is subdivided into four parts:

5.10.1 Observation single points

Observation points can be inserted where contaminant breakthrough or hydraulic-head values are to be monitored during the simulation. These points are also the basis for the reduced result data which are saved as ***.dar** files, if so selected in the **Control output data** menu of the **Simulator kernel** (Section 6.8). The number of observation points is unlimited. Observation points can either be set on nodes or arbitrarily within the model domain. Different import and export functions are available. A special **Point property** dialog allows you to define additional properties for the observation points.

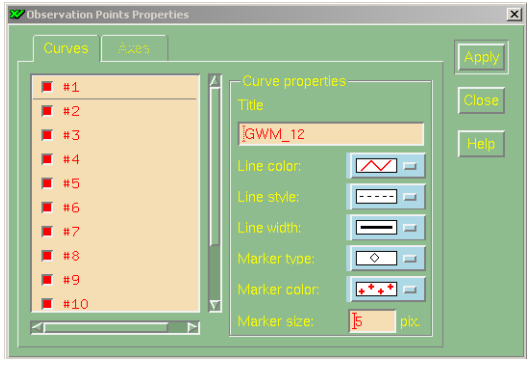


Figure 5.17 Observation points properties dialog.

Line style, width and colors of a line and markers refer to the diagrams in the simulator menu. An individual title can be assigned to the observation points. The observation point number is automatically changed by deleting points. For the use of the options please refer to the online **Help** hitting <F1> in the menu.

5.10.2 Observation point groups

Grouped balance points are groups of observation points for which balance fluxes will be computed during simulation. This option is useful for making a history of flow balances, e.g., for a river along its course. You can specify which fluxes should be considered, i.e., boundary fluxes, areal fluxes (groundwater recharge) or the sum of both. In order to define exactly for which nodes the budget will be analyzed you can set points only on nodes, not arbitrarily on elements. Each balance point group is identified by an unique group identifier. Using the **Point-joining** option the grouped balance points will be set on the nodes which are nearest to the imported points or lines. During the simulation, a **Balance flux** window will appear. You can view and save the balance data by activating the **Diagrams** option of the **Halt and view results** menu of the **Simulator kernel** or simply by clicking with the right mouse button on the diagram window (Section 6.4).

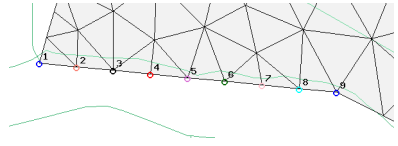


Figure 5.18 Observation point group.

5.10.3 Fences (sections)

Fences represent a specific arrangement of data and can be used for many purposes, for example, as line segments for a diagram evaluation in 2D, or to obtain cross-sectional displays in 3D. With this editor, you can create, load, export, and edit the fence segments or line sections you will need for the **Join** tool (Section 5.6), draw background maps as well as lines for cross sections, or lines and polygons for budget analysis of subregions and other postprocessing options.

5.10.4 Reference distribution

Reference distributions are used to compare the results of the simulation with given reference data such as the measured groundwater level. Each reference distribution is identified by a unique name. Values for a reference distribution are specified using the input tools described in Section 5.6.

5.11 Discrete Feature Elements

5.11.1 Basics

1D or 2D discrete-feature elements can be inserted interactively for the modeling of flow, mass and heat transport processes. Different laws of fluid motion can be defined for discrete-feature elements: Darcy, Hagen-Poiseuille and Manning-Strickler.

Discrete-feature elements represent finite elements of lower dimensionality which can be inserted at element edges and faces, or between nodes, of an existing mesh. They are useful to describe fractures in rocks, faults, boreholes, tunnels, rivers, channels, mining rooms and slopes, drainage elements, overland flows and others.

For detailed information on the theoretical background see the part of the FEFLOW White Papers called 'Discrete feature modeling of flow, mass and heat transport processes by using FEFLOW'.

5.11.2 Fracture editor

For the process of inserting, editing and deleting fracture elements a new 'Fracture Editor' is provided.

To enter the 'Fracture editor' click the new menu entry 'Discrete feature elements' in the 'Problem editor' menu.

The design of the 'Fracture editor' is similar to the other FEFLOW editors, containing different items at the top, the Mesh Inspector button, the tool switch, tool options, and a return button:

Use the 'Discrete element' button to assign fracture elements interactively at the screen after having set the corresponding properties.

The 'Delete' button allows to delete elements by clicking them with the mouse in the working window.

There are different types and modes of discrete elements. A type and mode set always consists of two activated buttons, one of the first block (violet buttons, type) and one of the second (turquoise buttons, mode).

Table 5.5 Discrete feature elements: types and modes

	Linear 1D element: Use this option to assign one-dimensional linear elements, e.g., to represent ducts or channels.
	Trilateral 2D element: Switch to trilateral elements to insert horizontal areal elements using triangular meshing, e.g., for horizontal fractures.
	Quadrilateral 2D element: Assign quadrilateral elements for horizontal fractures in quadrilateral meshes or for vertical fractures.
	Horizontal element[a]: Horizontal elements connect adjacent nodes in one slice (1D) or represent fractures parallel to the slice (2D).
	Vertical element: Vertical elements connect corresponding nodes at two adjacent slices (1D) or represent vertical fractures (2D).
	Arbitrary element: Use this element type to connect arbitrary nodes within the same slice. Only 1D arbitrary elements are currently implemented.

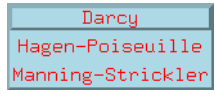
a.'Horizontal' means slice-parallel

With the exception of arbitrary elements, all fracture elements are set along finite-element edges (1D elements) or along finite-element faces (2D elements).

Vertical finite elements are set with respect to a given layer. For example, to assign a vertical tube between slice 3 and 4 the 1D vertical element has to be set on layer 3. It is indicated by the symbol ○.

The fracture elements can be assigned by using the **L-Join** or the **A-Join** Tool. It is also possible to copy all fracture elements between layers using the **Copy** tool.

Three different laws are available for the calculation of flow and transport along the discrete elements:



Each of the laws needs the specification of some material parameters. Use the buttons to switch between the parameter sets for flow, mass or heat transport.

All parameters have to be filled in the corresponding input boxes before setting a discrete element. It is possible to use different laws for different discrete elements in one FEFLOW model.

Besides 'Assign', joining tools for lines (L-Join) and polygons (A-Join) are available to enter and edit the discrete-feature elements.

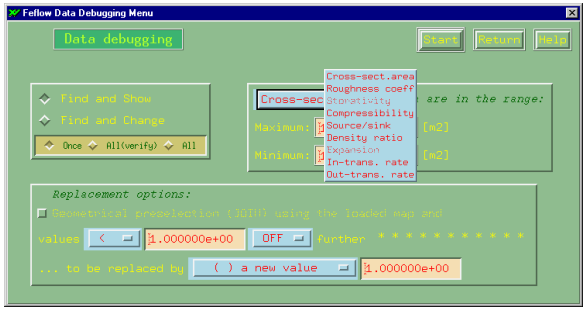


Figure 5.19 Data debugger for discrete feature elements.

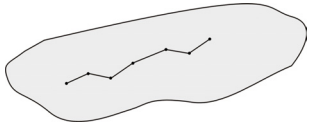
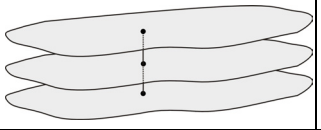
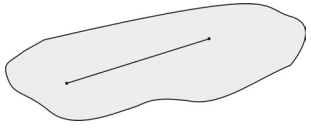
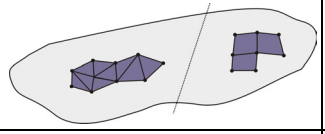
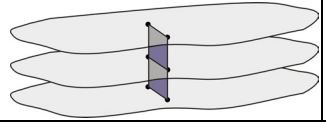
Changing parameters is possible via the 'Debug' tool. Please note that 'Debug' only affects the elements of the selected type and law. The material has to be chosen before starting the debug function. The parameter to debug is selected within the debug window.

The 'Convert' tool provides conversion functionality from one law to another.

5.11.3 Examples

Table 5.6 shows an overview of practical applications of discrete-feature elements in a FEFLOW model. Recommendations are given for the use of the different element types, modes and laws provided by FEFLOW.

Table 5.6 Examples for the application of discrete feature elements

Type	Mode	Sketch	Examples	Recommended law
			Open channel, river, stope channel or drainage trench filled by porous material	Manning-Strickler Darcy
			Borehole, shaft, abandoned well (open) borehole, abandoned well (filled by porous material)	Hagen-Poiseuille, Manning-Strickler Darcy
			Pipe, tunnel	Manning-Strickler
 			Horizontal fault overland flow, runoff drain section	Hagen-Poiseuille Manning-Strickler Darcy
			Vertical fracture or fault drain element, pervious shell	Hagen-Poiseuille Darcy

5.12 Problem Summary

The Problem Summary window is described in Section 4.9. It summarizes both the important data generated and the status of the problem-editing process. Select this tool to check the completeness of the data. See Section 4.9 and FEFLOW online **Help** for a detailed explanation.

5.13 IFM Modules

A 'Module selection' pop-up window allows to activate/deactivate program modules previously configured in the **Interface manager** (IFM, Section 11).

Modules must be activated before they can be used during a session. You should deactivate a module before editing it in the **Interface manager**. See the section **Programming interface** (Section 11) for further information.

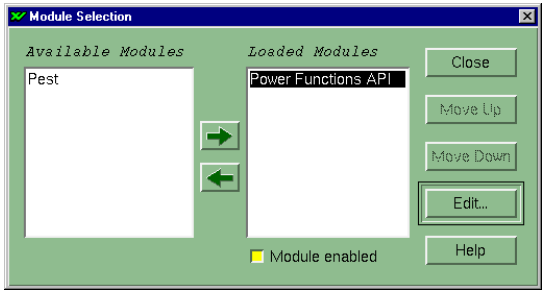


Figure 5.20 IFM Module Selection.

5.14 Mesh Geometry

Selecting this item invokes tools such as **Mesh enrichment**, **Delete elements**, **Check mesh properties** and **Triangularize quadrilateral elements**. See FEFLOW online **Help** for more details such as the inheriting of boundary conditions in case of mesh refinement.

Simulator Menu Items

6

6.1 Introduction

This section describes the executing, viewing and saving of flow and transport simulations. An option to go back to the **Problem editor** is also offered.

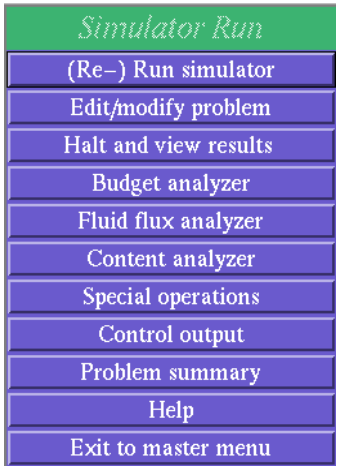


Figure 6.1 Simulator Run menu.

Upon invoking the FEFLOW **Simulation kernel**, the selected equation solver is started. Accordingly to the problem to be solved and the selected solver options (Section 2.6) various steps are required to prepare the numerical simulation.

The simulator dynamically allocates all data and working arrays needed for the simulation. If insufficient memory is available, an alert box appears and the simulator stops. Otherwise, the simulation continues with preparation steps: computing outer border mesh logics, and opening the simulator submenu with different windows to display results.

Select **Exit to master menu** to leave the simulator and enter the FEFLOW Shell. If you try to restart the simulator from the Shell for the same problem, the simulation will start from the beginning. However, it uses the resulting distributions for hydraulic head, contaminant mass and temperature from the last time as the new initial conditions.

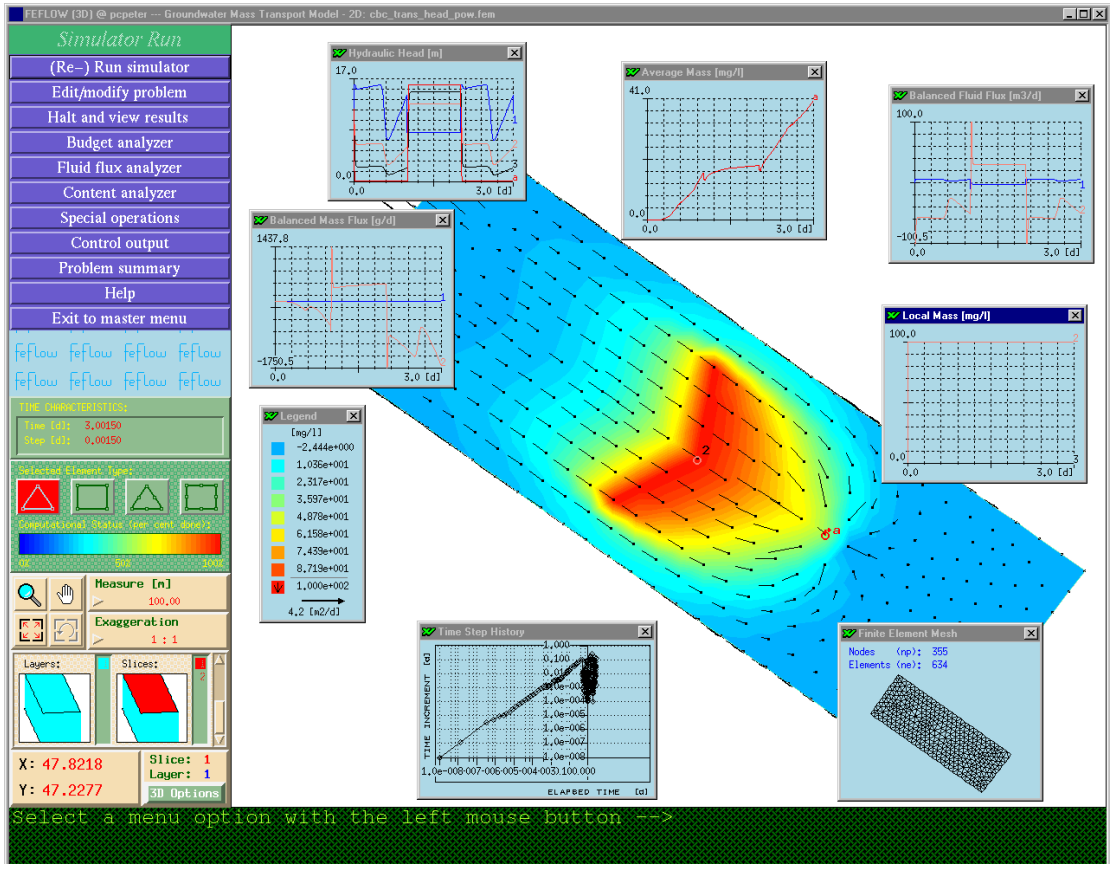
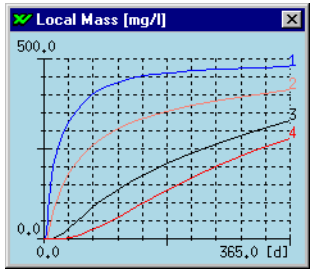


Figure 6.2 Simulator run.

6.1.1 Diagrams

Depending on the selected problem class, overlapping windows may be opened to visualize the progress of the simulation run. For a flow problem, there are three standard windows to display: the **Mesh**, the **Time history of hydraulic heads** (can be switched to pressure, moisture content or saturation) at the observation points, and the **Legend**.



For combined flow and transport problems, additional windows are available: the **histories of averaged concentration** at adjacent flux-occupied boundary sections (galleries, wells) and **the breakthrough curves of concentration at the observation points**.

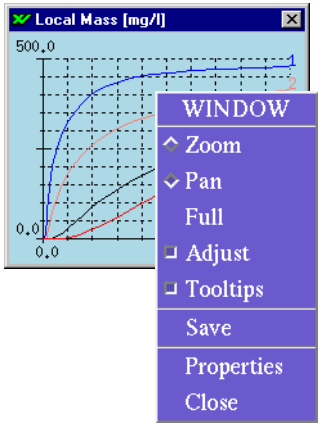
For nonlinear simulations (density-coupled, unsaturated flow, unconfined aquifers), using a (Picard) fixed-point iteration scheme (for steady-state or transient problems without predictor-corrector time-stepping), an additional window, **Error norm history**, is automatically opened to follow the progress of the successive iterative solutions. It contains a plot and numerical output of the error norm history. In case of automatic time-step control the **Time-step control** window is opened to plot the evolution of computed time steps during the simulation. The windows can be moved, resized, or closed at any time during the simulation. Notice, however, that to maintain efficiency, the manipulated windows are updated infrequently, i.e., some numerical (inner) loops have to finish before the windows are refreshed. The optimal time for window manipulation is when the simulator halts

- at the beginning and the end of a run, or
- if the simulation is interrupted between time-steps.

The **Log messages** window opens automatically if warnings or error messages are produced during the simulation session. The messages can be saved to a text file by clicking the right mouse button in the diagram.

All the diagrams are completely customizable. It is possible to define the axes, to change the scaling and even to underlay the diagrams with imported graphs or analytic functions so that computed results can be compared with measurement data already during the simulation.

6.1.1.1 Diagram menu



A right-click on any of the diagrams invokes the diagram menu. The following entries are available:

•**Zoom**: Switches to Zoom mode; the zoomer functions for the diagrams are similar to the FEFLOW zooming tool.

•**Pan**: Switches to Pan mode.

One of these two modes is always active. The Zoom mode is indicated by a magnifying glass for the cursor while a hand is shown in Pan mode.

- **Full**: The diagram scaling is adjusted to the full extent of the curves.
- **Adjust**: If Adjust is selected the diagram scaling is adjusted to new values when changes occur (e.g., during simulation run).
- **Tooltips**: Choose this option to show single curve values as tooltips when moving the mouse arrow over the curves.
- **Save**: Save the curve data in *.pow format.

- **Properties**: Invokes the 'FEFLOW diagram properties' window described below.
- **Close**: Use this option to close a diagram window. To show the window again go to the Quick access menu and use the 'Window' function.

The default settings in the diagram menu are as shown in the image above.

6.1.1.2 FEFLOW diagram properties

Choosing 'Properties' from the diagram menu a new window is opened offering all tools for customizing the diagram. There are two tabs for editing the curve properties and the properties of the axes.

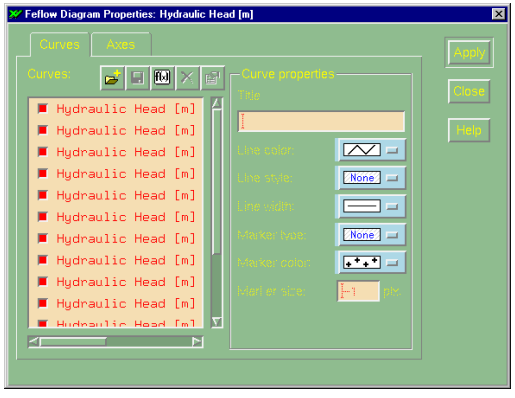


Figure 6.3 Diagram properties - curves tab.

Curves

At the top of the window some buttons are placed for adding and removing curves as well as for saving and loading them:

Table 6.1 Diagram properties - buttons

	Add a curve loaded from a file: Load one or several curves in *.pow file format.
	Save a curve to a file: Save the selected curve to a *.pow file.
	Add a curve based on an expression: Opens the 'Analytical expression editor' for adding analytical functions. See detailed description below.
	Delete the curve from the diagram: Remove the currently selected curve(s) from the diagram.
	Edit special curve properties: Invokes the 'Analytical expression editor' for editing an analytical function. See detailed description below.

In the left part of the window an overview of all curves is shown. Use the square to the left of the curve name to show or hide a curve in the diagram.

The settings to the right always refer to the curve currently selected in the list. Please note that for changing the properties only one curve may be selected.

In the 'Title' input field you can specify the curve title to be shown in the diagram. Beneath the title there are five switch toggles and an input field. Their functions are as follows:

Table 6.2 Diagram style settings

	Line color: Set or change the color of a curve in the diagram.
	Line style: Define whether a curve should be shown solid, broken or dotted.
	Line width: Specify the with of the line.
	Marker type: State whether markers should be shown and set the marker aspect.
	Marker color: Specify the color of the markers.
	Marker size: Define the size of the markers in pixels.

Analytical expression editor

In this window, which is invoked by the f(x) button, analytical expressions can be prepared for the use as diagram curves. Besides the basic arithmetic operations scientific mathematics are possible, too. All functions have to be written for x as argument. See the online Help for a detailed list of operators.

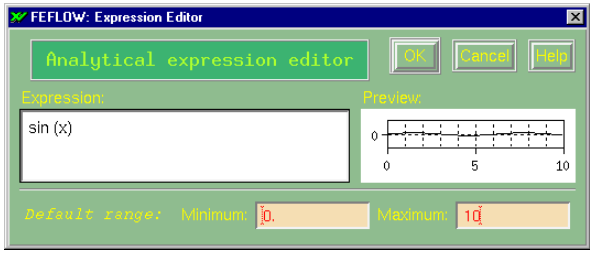


Figure 6.4 Analytical expression editor.

Axes

The second tab in the diagram properties window provides the possibility to customize the diagram axes.

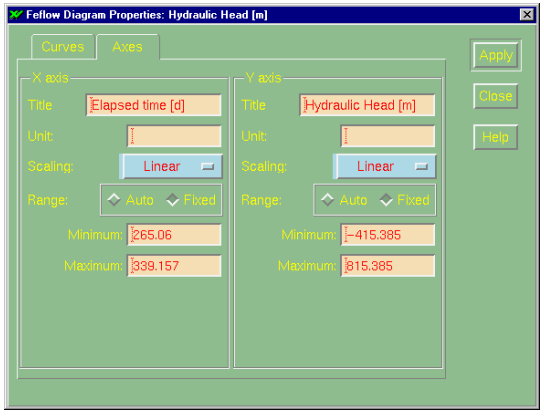


Figure 6.5 Diagram properties - axes tab.

The settings for the abscissa ('x-Axis') are located in the left part, the ones for the ordinate ('y-Axis') in the right part. Title and unit describe the labeling of the axes. The scaling of both axes can be set individually, either to 'Linear' or to 'Logarithmic'. The shown range of values is automatically adapted to the currently shown functions by default ('Auto'). Alternatively it can be 'Fixed'. In the latter case the minimum and maximum values have to be specified.

6.1.2 Legend editor

The legend editor supports the user-defined settings for fringed isolines and vector drawings. It can be invoked by right-clicking the legend window and choosing 'Edit' from the pop-up menu.

Several settings can be made:

- Resolution - number of colors used
- Minimum / Maximum - min./max. values for fringes
- Scaling - linear or logarithmic
- Copy to custom - in custom mode the scaling of the legend can be edited manually
- Import / Export custom - open and save legend files (*.leg)
- Rainbow directions - select the direction of the color scheme
- Drawing options - invokes the drawing options menu
- Velocity vectors - drawing of velocity vectors can be turned on and off and can be changed from linear to logarithmic scaling

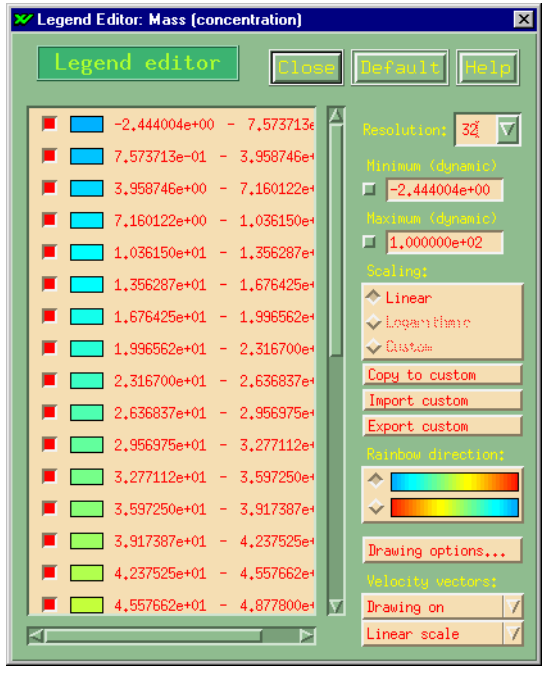


Figure 6.6 Legend editor.

6.2 (Re-) Run Simulator

Selecting this command the simulation is executed. All major simulator actions are described by messages in the message bar on the lower part of the screen. The progress of the computation steps can be observed on the **Computational status** bar.

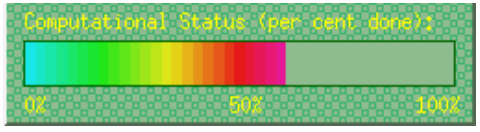


Figure 6.7 Computational Status bar.

The simulator updates the current flow velocity pattern and/or mass fringed isolines whenever new results are available. The update frequency can be limited by setting the number of time steps between updates to a value greater than one (see Section 6.8). After each time step, the simulation can be interrupted by hitting the **<Esc>** key or pressing the right mouse button. When the simulation is interrupted, different menu items or window manipulations are available.

The simulator can easily be restarted by clicking on **Re- (Run) Simulator** again. A restart is possible even when the final time has been reached. In this case, the simulator continues from the final stage and automatically increases the absolute initial time.

The simulator uses an automatic resolution control to reduce numerical effort during the solution of the governing equation systems. Depending on problem class and time-step behavior, the control can turn the equation assembly or the decomposition/factorization on or off. For constant time steps in linear transport processes, the matrix assembly and factorization of the equation systems are executed only for the first time step, while all subsequent time levels can be quickly solved by the fast resolution procedure. The resolution control is also maintained if the simulation is interrupted.

If a problem is ill-posed, warnings from iterative equation solvers (default option) may be produced during the preconditioning phase. These warnings indicate that poor convergence is to be expected and that the simulation will potentially fail.

6.3 Edit or Modify Problem

This option starts the **Problem editor** to modify the current problem. It allows you to restart the analysis quickly and simply under modified conditions suitable for alternative solution and scenario analysis. For transient problems the information of the last time step is saved to ensure an easy restart of the simulation. For more details, refer to the Problem Editor menu options (Section 5).

6.4 Halt & View Results

The **Halt and view results** dialog allows viewing and exporting of the resulting parameter distributions and velocities after the simulation has finished or when it has been interrupted. The following options are available to view and analyze the computational results at the given time level. The dialog is identical to the Results Viewer in the **Postprocessor** menu.

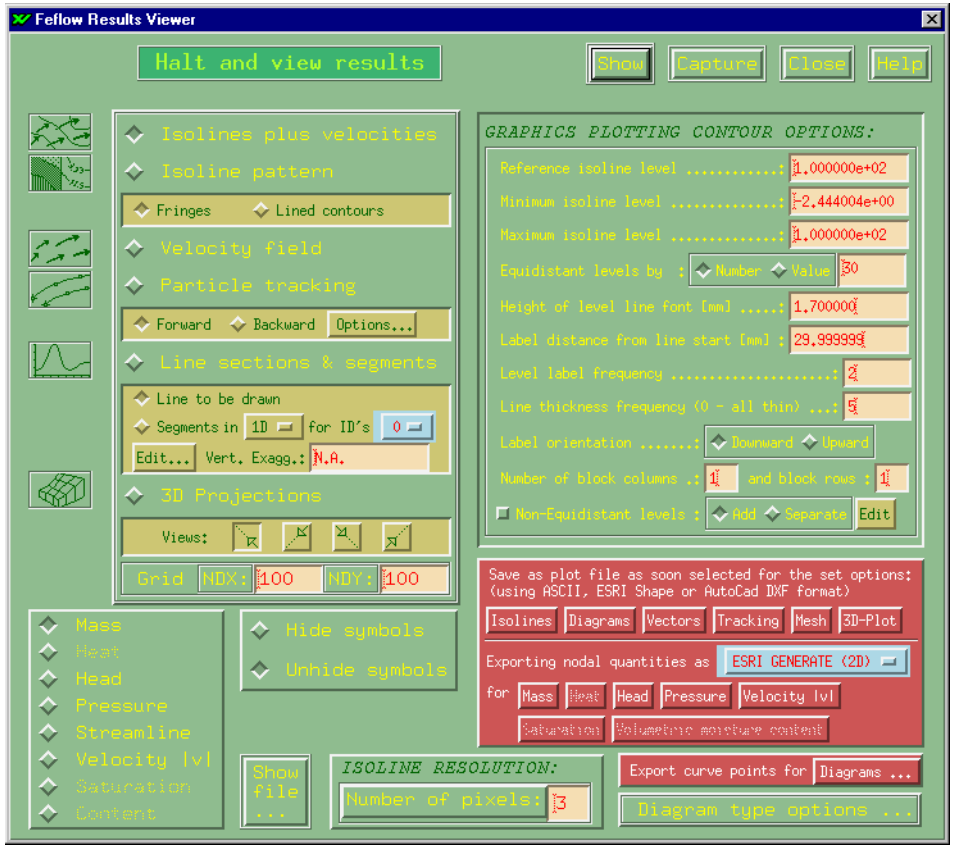


Figure 6.8 Halt and view results dialog.

6.4.1 Visualization

The Results viewer supports
- isolines and fringes
- velocity vector fields
- particle tracking
- cross sections along lines and segments
- pseudo 3D-projections

to visualize the current distributions. Select the parameter you want to visualize (lower left part of the menu), define the visualization mode and click on the **Show** button for creating the view. You can analyze the hydraulic head, pressure, saturation, moisture content, contaminant mass, temperature and velocity distribution, and streamlines. Submenus like the **Pathline selector** can be activated for special settings. See the online **Help** for detailed information.

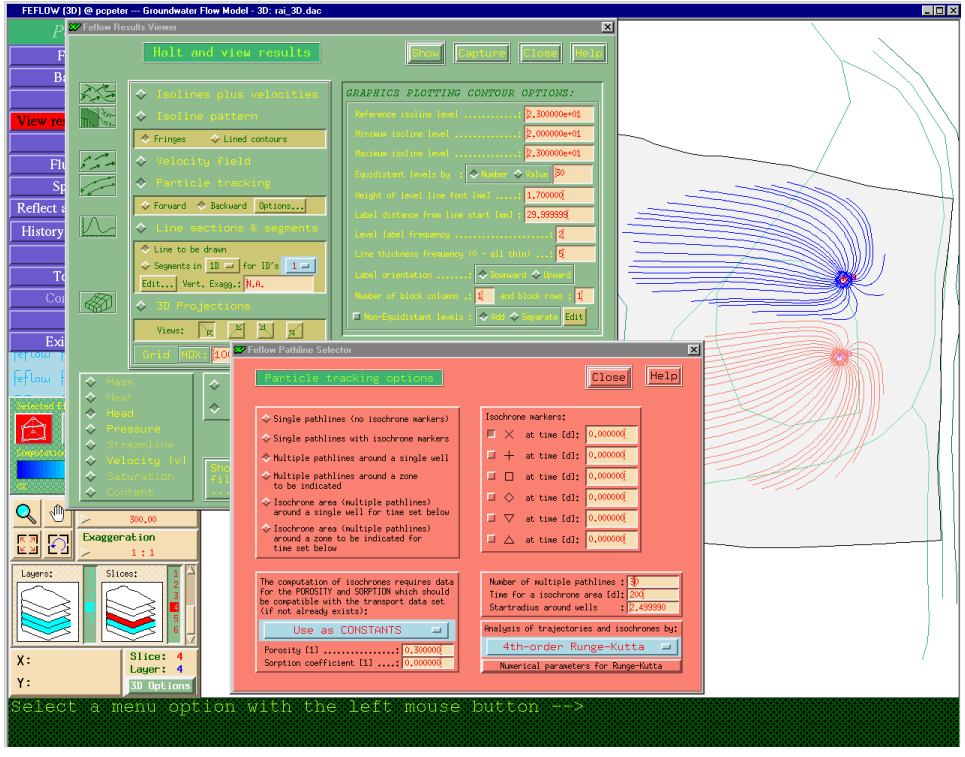


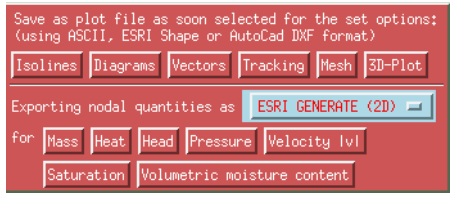
Figure 6.9 Pathline selector, Halt and view results window.

6.4.2 Data export

The easiest way to export data in form of georeferenced plots is using the **Capture** button instead of **Show**. The plot is added to a plot stack. When FEPLOT is started using the **Print...** button in the Quick Access menu or in the Shell File Menu the plots on the stack are recognized by FEPLOT as georeferenced map objects.

Using the capture function on a UNIX system the plot will be stored as *.plx file. This format can be read by the Windows-based **FEPLOT** tool.

Different plots can be stored in one map object as layers to ensure an exact overlay of the objects. FEFLOW plx files, ESRI shape files, ARC/INFO compatible ASCII (Generate) files and AutoCAD dxf data can be visualized in the same map object. All map objects are georeferenced. Conforming to GIS style, the classification settings of the maps can be changed based on the corresponding attribute data. The definition of templates for default layouts is supported. UNIX users may install FEPLOT on a PC and import ESRI shape files or FEFLOW plx files from their UNIX environment. FEPLOT is described in more detail in the Tutorial (see Section 10.3.5).



Different data formats for the export can be specified using the options in the lower right part of the **Halt & view results** menu: The menu items shown in red color refer to the plotting and exporting of computed results. In the upper part of the red square there are six buttons for different types of graphics plot output. The displayed data can be stored in the ARC/INFO compatible ASCII Format (lines and grids), in the ArcView Shape file format, as .dxf file, or as FEFLOW-specific .plx file for visualization in **FEPLOT**. Spatial data are accompanied by attribute data in ASCII, INFO or dBase format. You can define file formats and unit conversions in the **Data store manager**, which is accessible via the '**Configure**' button in the FEFLOW **File selector** menu. Diagrams are stored in .fpd files which can be read by XPLOT, the FEFLOW plotting tool in UNIX environments.

For additional and more detailed information please activate the FEFLOW online **Help** by hitting <F1> or by clicking the **Help** button

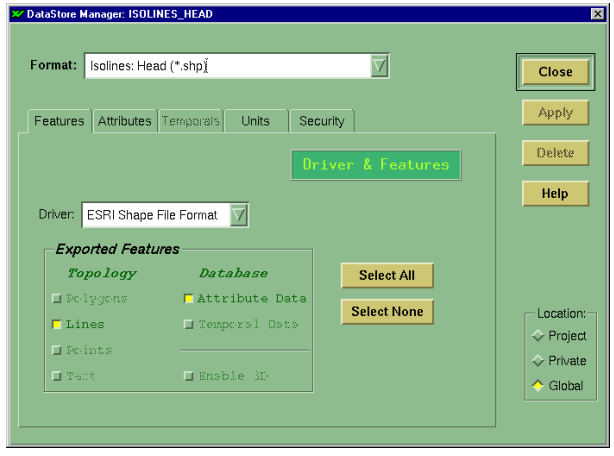


Figure 6.10 Data Store Manager (DSM).

The toggles and entries of the previous menu items are also valid for export. For example, if mass is set, then a isoline map will refer to the computed mass distribution.

The output of resulting nodal quantities for all parameters can be performed in different ASCII formats using the buttons in the lower part of the red box. For more detailed information see FEFLOW online **Help**.

6.5 Budget

Budget computes quantities of fluid masses, contaminant masses, and heat entering or exiting the simulated region, subregions or boundary sections, i.e., it computes balances for a quantity entering or leaving the model domain. The quantities for fluid, contaminant mass and heat are evaluated in an unified manner:

Imbalance

- Fluxes along outer or inner boundaries, e.g., borders occupied by Dirichlet, Neumann, or Cauchy boundary conditions (first, second, and third type)
- Injections and withdrawals through single wells (fourth type)
- Areal fluxes due to infiltration, recharge, leakage etc.
- Imbalance: Gain(+)/Loss(-)

Boundary conditions

- Fluxes along outer or inner boundaries occupied by Dirichlet (first type) boundary condition
- Fluxes along outer or inner boundaries occupied by Neumann (second type) boundary condition
- Fluxes along outer or inner boundaries occupied by Cauchy (third type) boundary condition
- Injections and withdrawals through single wells (fourth type)

Inputs (fluxes in) to the areas or border sections are counted as positive, outputs (fluxes out) as negative quantities. The imbalance corresponds to the sum of all entering and exiting amounts:

Imbalance =
BorderIn + BorderOut
+ WellIn + WellOut
+ ArealIn + ArealOut

A positive imbalance implies a gain, e.g, storage in the aquifer at transient conditions. A negative imbalance indicates a loss in the (sub)region, which can occur during transient dewatering or retardation in the aquifer. For steady-state conditions, the remaining imbalance for a total balancing over the entire region represents a measure of the computational accuracy. For more details and the meaning of balancing for different transport formulations (convective or divergence forms) and their different boundary conditions refer to the Reference Manual.

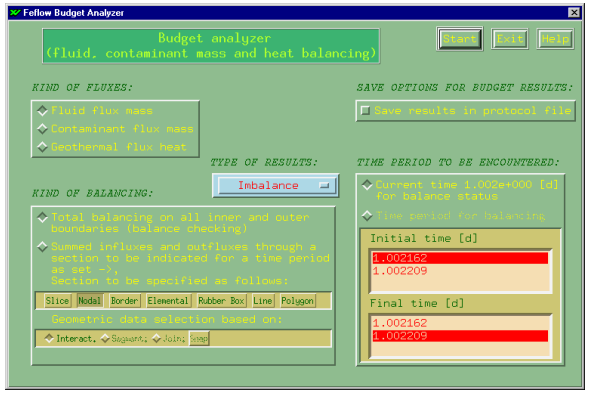


Figure 6.11 Budget analyzer.

***Notice**: The quantities computed by the Budget analyzer are defined as positive for influxes, negative for outfluxes. This is contrary to the definition of the boundary conditions!*

***Notice**: The meaning of 'fluxes' depends on the selection between Convective form transport (default) and Divergence form transport in the Options menu of the Shell. For the former, fluxes are dispersive, i.e., they are controlled only by the concentration gradient. For the divergence form, the total fluxes consist of the convective and dispersive parts. Please refer to the FEFLOW White Paper 'About the difference between the convective form and the divergence form of the transport equation'.*

The fluid, contaminant and heat budgets are computed based on the integrated-discretized balance equations using the *Continuous Boundary Flux Method (CBFM)* of evaluating the fluxes at the best accuracy.

The **Budget analyzer** menu (Figure 6.11) contains a number of options. Use the toggles to select between fluid flux mass, contaminant flux mass and geothermal flux heat. **Fluid flux mass** results in the balancing of the flow equation. **Contaminant flux mass** results in the balancing of the mass transport equations. **Geothermal flux heat** results in the balancing of the heat transport equations. Subareas for balancing may be defined interactively by digitizing polygons on the model area or by importing background maps as templates.

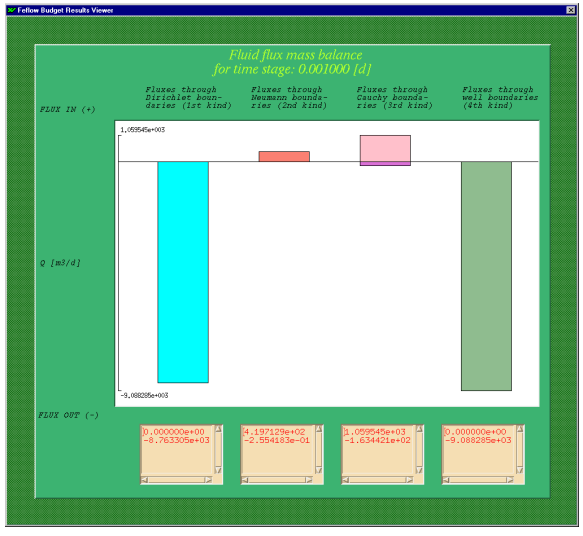

Fluid flux mass balance
for time stage: 0.001000 [d]
Fluxes through Dirichlet boundaries (1st kind)
Fluxes through Neumann boundaries (2nd kind)
Fluxes through Cauchy boundaries (3rd kind)
Fluxes through well boundaries (4th kind)
FLUX IN (+)
Q [m3/d]
FLUX OUT (-)

Figure 6.12 Budget output.

Two different options exist to select times and time periods that are to be used in the balance computations:

Current time... [d] for balance status

The balance computations are for the current time (at which the simulator is paused). The results represent fluid fluxes Q, contaminant fluxes Q_c or thermal fluxes Q_t. The corresponding units are [m^3/d], [g/d], [J/d], respectively (Figure 6.12).

Time period for balancing

This option is accessible from the **Postprocessor**. It is not accessible from the *Simulator Kernel* because there only the current time stage is available. To analyze a time period, the simulation run has to be stored in a **Postprocessor** file (use the **Control output** menu (Section 6.8) for this purpose). The **Postprocessor** allows a budget analysis for a simulated time period. The time histories of the fluxes (Q [m3/d], Q_c [g/d], Q_t [J/d]) and the fluid masses M [m^3], contaminant masses [g] and thermal energy [J] accumulated during the selected time period are computed as results.

All results of the different budgeting operations can be stored in a **Protocol file**. Moreover, all **Accumulated nodal fluxes** can be saved to an ASCII file. For each selected node the boundary flux is symbolized by red circles for influxes and blue circles for outfluxes in the working window, where the diameter of the circles is related to the flux quantity.

Detailed information about the **Budget analyzer** is provided in the online **Help**.

6.6 Fluid Flux Analyzer

The **Fluid flux analyzer** tool computes quantities of horizontal or vertical fluid fluxes entering or exiting the simulated region, subregions, points, or boundary sections. It is not intended as a check on numerical accuracy, but rather as an additional tool for evaluating computed distributions of the **Darcy velocity** and related discharge quantities from this velocity distribution.

The flux through an area (defined by a geometric section) will generally be computed by subdividing the section into many small (vertical or horizontal oriented) line segments. The integrated flux represents the normal flux through the line (polygon) segment. The flux unit is 'volume per time'.

Please note that the results of the Fluid Flux Analyzer are not exact flux values. Inaccuracy may result because

- velocities are secondary results of the simulation run
- the velocity vectors from nodes are projected on sections

However, it is a useful tool for estimating fluxes between subregions in your model domain, e.g., flux into an open pit from the surrounding aquifer or fluxes through a cross section.

For more detailed information see the Reference Manual and the online **Help**.

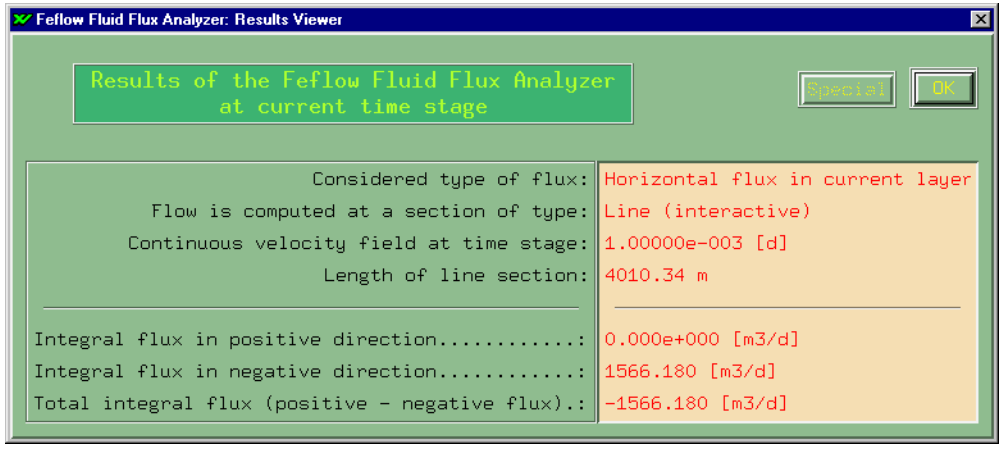


Figure 6.13 Fluid flux analyzer.

6.7 Special Operations

This menu allows difference operations on the resulting data or between resulting data and reference data for the creation of difference maps.

Two tabs are available:

Spatial

- No spatial operation or reset and retrieve original data
- Difference: top minus head
- Difference: head minus bottom.

The operations are applied to hydraulic head only. All visualization methods of the **Results viewer** (Section 6.4) may be used for analyzing the difference distribution. To retrieve the original data enter the special operations window again and choose the first option (no spatial operation).

Reference

Applies difference operations between computed results and reference distributions assigned before in the Reference distribution menu (Section 5.10).

Choose **Difference: Computed distribution minus selected reference** to compare the computed distribution and the selected reference distribution. If no reference distribution has been assigned this option is not available. To return to the computed values select **No reference operation or reset and retrieve original data.**

6.8 Control Output

This menu controls the saving modes for the computation results and the display of the current results during the simulation.

The upper section **Data to file** manages the saving of data to a file:

- **Record reduced data (ASCII)** - Observation-point data only are recorded to a ***.dar** file.
- **Record complete data (ASCII or binary)** - Data are recorded to a ***.dac** file. This option saves the complete data as needed by the **Postprocessor**.

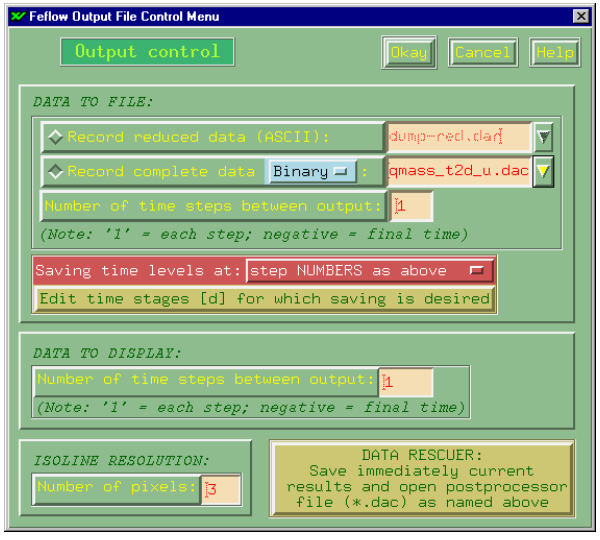


Figure 6.14 Output control.

Further options are available to select the *Time steps between output* or edit *fixed time stages* for which saving is desired.

The **Data rescuer** option can be used to save the

current results in a postprocessor (*.dac) file.

The **Data to display** section controls the update frequency for the visualization of results during the simulation by specifying the number of time steps between subsequent redrawings. The isoline resolution defines the accuracy of fringe isoline drawings for quadrilateral meshes. For more detailed information see the online **Help**.

6.9 Problem Summary

This option summarizes the status of problem editing. Select this submenu to check problem data for completeness and consistency. Section 4.9 describes the corresponding popup window in detail.

Feflow Problem Summary
Problem Summary
Okay
DESCRIPTORS:
FILE NAME .....: dynamic_river.fem (DEMO DATA 4.626)
PROBLEM TITLE .....: Exmpl.:lin.1D-interpol. NO timelevels
RECENT UPDATING .....: Mon Aug 06 14:05:56 2001
DIMENSION .....: Two-Dimensional
TYPE .....: Saturated
NUMBER OF LAYERS .....: Inconsiderable
NUMBER OF SLICES .....: Inconsiderable
PROBLEM MEASURE .....: 8143.20 [m]
VERTICAL EXAGGERATION : 1.00 : 1
PROJECTION .....: Horizontal (unconfined/phreatic aquifer)
PROBLEM CLASS .....: Separate flow process
TIME CLASS .....: Unsteady flow
TIME STEPPING SCHEME .: Adams-Bashforth/Trapezoid rule (AB/TR) predictor-corrector
UPWINDING .....: No upwinding (best-accurate Galerkin-based formulation)
MESH DATA:
ELEMENT TYPE .....: 3-noded triangle
MESH ELEMENTS ....: 549
MESH NODES .....: 314
MESH OPTIMIZATION : Not done
FLOW CONDITIONS:
BOUNDARIES .....: Specified Unspecified
INITIALS .....: Specified Default
MATERIALS .....: Specified Default
READY TO RUN ?
Yes
No
TRANSPORT CONDITIONS:
BOUNDARIES .....: Specified Unspecified
INITIALS .....: Specified Default
MATERIALS .....: Specified Default

Figure 6.15 Problem summary.

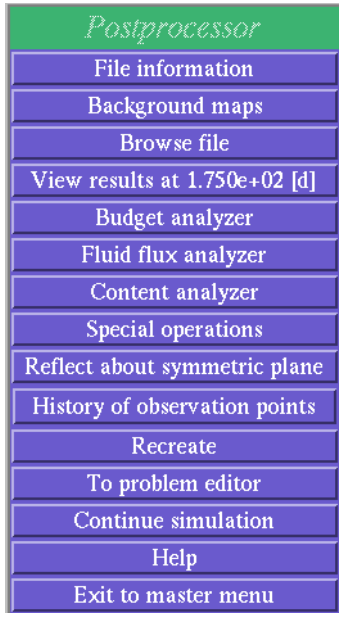
6. Simulator Menu Items

Postprocessor Menu Items

7

7.1 Introduction

The **Postprocessor** contains a number of options and capabilities which are useful for studying and evaluating computational results. The **Postprocessor file** is selected in a **File selector** box. The **Postprocessor** reads ***.dac** files which have been produced during a (previous) simulation run.



A menu appears after a ***.dac** file has been loaded. When invoked, the **Postprocessor** inspects all saved time steps. After the loading phase, it halts at the last time-step. The **Postprocessor** displays the same diagram windows as the **Simulator** (see Section 6.1). For transient problems only the values of the saved time steps appear in the diagrams. If only selected time stages have been saved in the postprocessor file, curves may appear "step-like".

The **Postprocessor** offers numerous menu items which are described in detail below.

7.2 File Information

This window summarizes all important data of the selected **Postprocessor** file, e.g. **File name**, **Problem title**, **Date of file data**, **Problem dimension**, type of **Projection**, etc. You should select this option to check problem data.

7.3 Background Maps

You can use this option to enter the **Add map...** and the **Map manager** options, which are identical to the options of the same name in the Shell **File** menu (Section 2.2).

7.4 Browse File

Notice: The browser can be used simultaneously with other menu items. For instance, the Results Viewer can remain open while a different time stage is selected in the browser.

A scroll list appears when this option is selected. All time steps scanned from the postprocessor file are listed in ascending order. The currently selected time step is highlighted in red color.

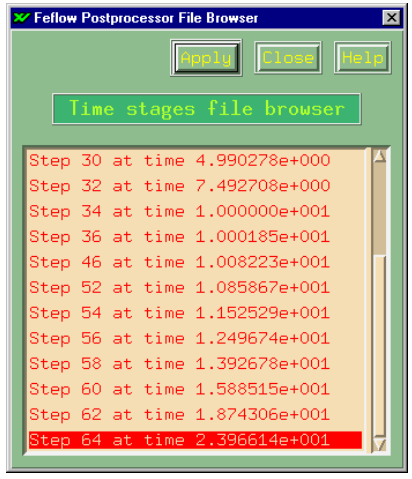

Feflow Postprocessor File Browser
Apply
Close
Help
Time stages file browser
Step 30 at time 4.990278e+000
Step 32 at time 7.492708e+000
Step 34 at time 1.000000e+001
Step 36 at time 1.000185e+001
Step 46 at time 1.008223e+001
Step 52 at time 1.085867e+001
Step 54 at time 1.152529e+001
Step 56 at time 1.249674e+001
Step 58 at time 1.392678e+001
Step 60 at time 1.588515e+001
Step 62 at time 1.874306e+001
Step 64 at time 2.396614e+001

Figure 7.1 File browser.

Initially, the last step of the simulation is selected. By using the browser, you can select different time levels for the **Postprocessor** evaluation. If you wish to change the current time level, select the corresponding list entry and press the **Apply** button. The **Cancel** button keeps the **Postprocessor** at the previous time level.

7.5 View Results at Current Time Level

Various postprocessor options are available to view and export the computational results at the selected time level. The **Results viewer** window corresponds with the **Halt and view results** window of the Simulator (Section 6.4). To end viewing, select the **Exit** button in the submenu.

For more detailed information, see the identical **Halt and view results** option of the **Simulator** menu (Section 6.4) or the FEFLOW online **Help**.

7.6 Budget

This item is identical to the **Budget** menu of the **Simulator** menu (Section 6.5), except that in the **Postprocessor** the budget can also be analyzed over time periods, displaying the flux quantities as diagrams for a simulated time period. The time histories of the fluxes (Q [m3/d], Q_c [g/d], Q_t [J/d]) and the fluid masses M [m³], contaminant masses [g] or energy [J] accumulated during the selected time period are computed.

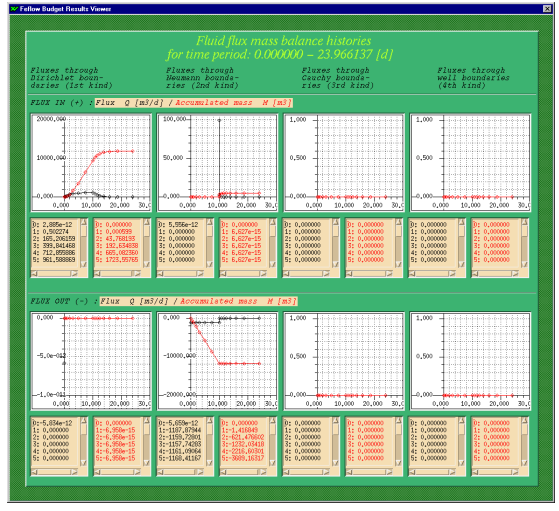


Figure 7.2 Budget Analyzer result.

7.7 Fluid Flux Analyzer

This item is identical to the one in the **Simulator** menu (Section 6.6), except that in the **Postprocessor** fluxes can also be analyzed over time periods.

7.8 Content Analyzer

The content analyzer is described in detail in Section 5.6.

7.9 Special Operations

This data-operator menu allows useful manipulation of the resulting data by various **Spatial**, **Reference**, and **Temporal** operations. Spatial and Reference operations are described in Section 6.7.

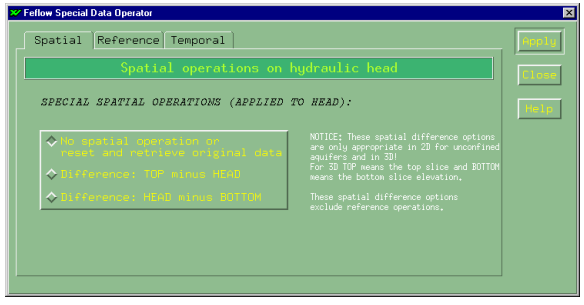

Fellow Special Data Operator
Spatial
Reference
Temporal
Apply
Close
Help
Spatial operations on hydraulic head
SPECIAL SPATIAL OPERATIONS (APPLIED TO HEAD):
No spatial operation or reset and retrieve original data
Difference: TOP minus HEAD
Difference: HEAD minus BOTTOM
NOTICE: These spatial difference options are only appropriate in 2D for unconfined aquifers and in 3D!
For 3D TOP means the top slice and BOTTOM means the bottom slice elevation.
These spatial difference options exclude reference operations.

Figure 7.3 Special operations.

The **Temporal** operations include differences, standard deviations or cumulative changes for time stages to be selected. The operations are applied to the hydraulic head, the contaminant and the temperature distributions; all other results are not affected. Two accompanying scroll lists contain all available time stages. The following toggles set the corresponding types of operations:

No temporal operation or reset and retrieve original data

This default option resets all previous operations and retrieves the original data.

Difference first time minus second time as selected

In the scroll lists of this menu, you must select two time stages (the initial and the final times are default) for which the difference of the resulting data (hydraulic heads, concentrations or temperature) is to be computed.

The formula is written as:

$$Difference = Result_{(First\ Time)} - Result_{(Second\ Time)}$$

Standard deviation over a time period as selected

The population standard deviation for the time levels is computed over the time period selected in the scroll lists. With N denoting the number of selected time stages, the formula is:

$$SDev(x_1, \ldots, x_N) = \sqrt{Var(x_1, \ldots, x_N)}$$

with the variance:

$$Var(x_1, \ldots, x_N) = \frac{1}{N-1} \sum_{j=1}^{N} (x_j - \bar{x})^2$$

and the mean of the values $x_1, \ldots, x_N$:

$$\bar{x} = \frac{1}{N} \sum_{j=1}^{N} x_j$$

Cumulative changes over a time period as selected

This option displays the temporal sensitivity of the results as accumulation of absolute deviations for adjacent times over the time period selected in the scroll lists. The cumulative changes are computed according to the following formula:

$$Cum(x_2, x_N) = \sum_{j=2}^{N} |x_j - x_{j-1}|$$

Apply

Pushing the **Apply** button executes the selected operation type. The menu disappears and a red label in the **Postprocessor** menu indicates the current operation type. You can now select further menu items (e.g., **View results**) to study, visualize or plot the manipulated data. To reset or alter the operation, you can select the red push-button of the data operator again. Once the **Data operator** menu reappears, you can select further items. The easiest way to reset and retrieve the original data is to leave the operator menu via the **Exit** button after setting the toggles to the default "No temporal / spatial operation...".

7.10 Reflect About Symmetric Plane

This enables the reflection of the mesh (and all its data) about one or more reflection planes. If a computation utilized symmetric planes in the problem formulation, and if it is only necessary to model a part of the complete mesh, you may wish to evaluate and visualize the results on the full problem geometry. The reflection planes can be defined and the complete problem recreated by using this feature.

7.11 History of Observation Points

This button invokes a helpful submenu that allows to manipulate the number and position of observation points in order to draw modified history curves (breakthroughs).

A cascade menu offers four commands:

Select as nodes/points

Observation points can be set at nodes or arbitrary locations in the mesh.

Add further points and redraw

You have the choice of adding further observation points to the existing ones. As soon as this option is selected, the **Postprocessor** browses through the database and draws the new time history curves in the subwindows.

Delete all points before adding new one

All existing observation points are erased before

you can select new observation points.

Import points and add

Coordinates for new observation points can be loaded from a database.

Save data of points as *.dar file

This item is useful if you need the detailed numerical values of observation points. You have to select an output file name by the file selector where the point data of observation points in time are saved.

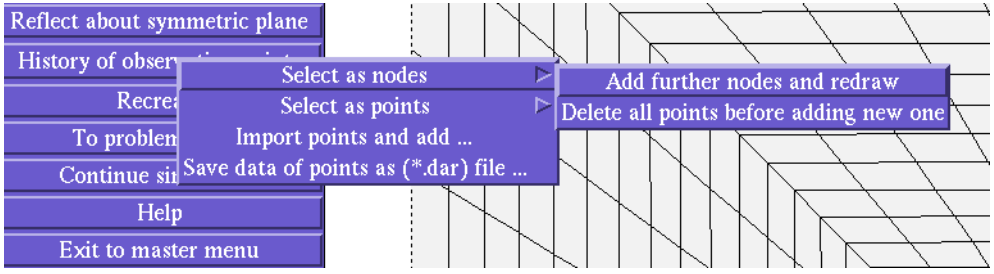
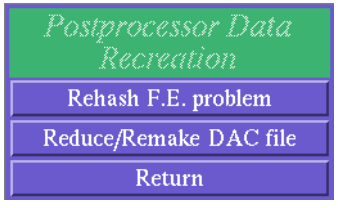


Figure 7.4 History of observation points menu.

7.12 Recreate



This command allows the recreation of a FE problem file from the **Postprocessor** database and the deletion of time stages in the postprocessor file. It is useful if you wish to continue a simulation using the last time level as the initial condition for the simulation run.

Rehash F.E. problem

If selected, a message window shows you the current time stage and asks for confirmation before creating a new finite-element problem based on the postprocessor data. If you accept these conditions, you can **Save** the data via a file selector. You can also leave the window via the **Cancel** button.

Reduce/remake DAC file

It allows the selection of time stages which are to be discarded. A new postprocessor file is created containing the reduced data set. Overwriting of the original DAC file is not possible.

***Notice**: In case of movable meshes in 3D, the stratigraphy of the last selected time step is maintained when exiting the Postprocessor, i.e., when returning to the master menu. To create a 3D problem file with the original stratigraphic data use the 'Rehash F.E. Problem' option.*

7.13 To Problem Editor

Use this option to enter the Problem editor (Section 5) for analyzing or re-editing the current parameter settings for the time step selected in the Browse File menu. Problem Class and Temporal & Control Data properties cannot be viewed or edited.

7.14 Continue Simulation

The simulation can be continued directly from the postprocessor. This is useful whenever the final time for which the postprocessor data were stored in a simulation run is later considered insufficient, or if a simulation that had been interrupted (e.g., by a system crash) is to be completed based on the already simulated results. The command **Continue simulation** starts the **Simulation kernel** (Section 6). You can define a new initial time step length, and a new final time for transient simulations. The new results are appended to the current postprocessor file (.dac).

The online **Help** offers a complete description of the Postprocessor. To leave the Postprocessor and enter the FEFLOW shell, the menu item **Exit to master menu** should be selected.

3D Options Menu Items

8

8.1 Overview

The 3D options menu offers several graphical tools for a 3D analysis of parameter distributions and for performing a 3D particle tracking. The menu is opened by clicking the green **3D-Options** button located at the lower left side of the working window.

Commands are available to visualize different parameter distributions in a 3D view, draw isosurfaces, cut the projection, and draw 3D pathlines. All actions are described in the message window at the base of the working window. The visualized objects can be rotated, moved and zoomed by mouse and keyboard control.

Clicking the 3D-Options button cascade menus appear:

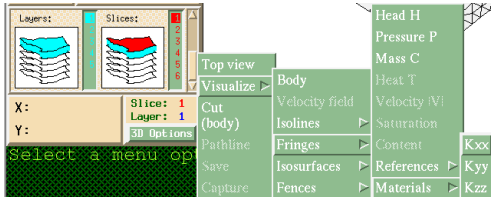
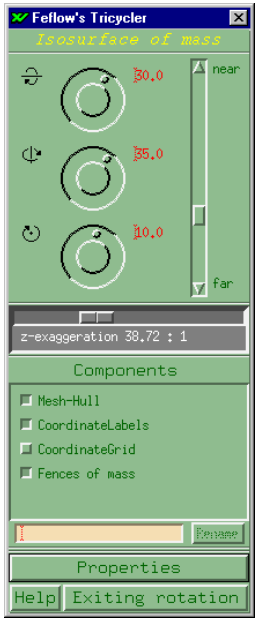


Figure 8.1 3D options menu.

8.2 The Tricycler

The FEFLOW **Tricycler** menu controls the rotation, zooming and z-exaggeration of the model projection. You can also zoom inside the body of the model (useful for checking the bottom elevation). Different components of the view such as isosurfaces or background maps can be turned on and off and can be given user-specified names.



The **Properties** button invokes a submenu where Isosurface levels (**General**), Drawing options (**Mesh**), and the shading colors (**Color**) can be set.

The Tricycler is visible during the whole 3D options session. Click on **Exiting rotation** to return to the 2D visualization; click on **Help** for detailed online **Help**.

Rotation and zooming of the body of the model is also possible via mouse and keyboard commands. The message bar below the working window displays the necessary information.

8.3 Visualize

You can visualize the model domain in 3D in different view modes:

- body,
- isolines,
- fringed isolines,
- isosurfaces and
- fences.

In each of the view modes one of the model parameters can be chosen:

- hydraulic head,
- pressure,
- mass,
- temperature,
- velocity,
- saturation,
- moisture content,
- reference distributions and
- material parameters (conductivity).

Some of the view modes can be combined; for example, you can visualize fringed isolines for the hydraulic head and add isosurfaces for the contaminant mass.

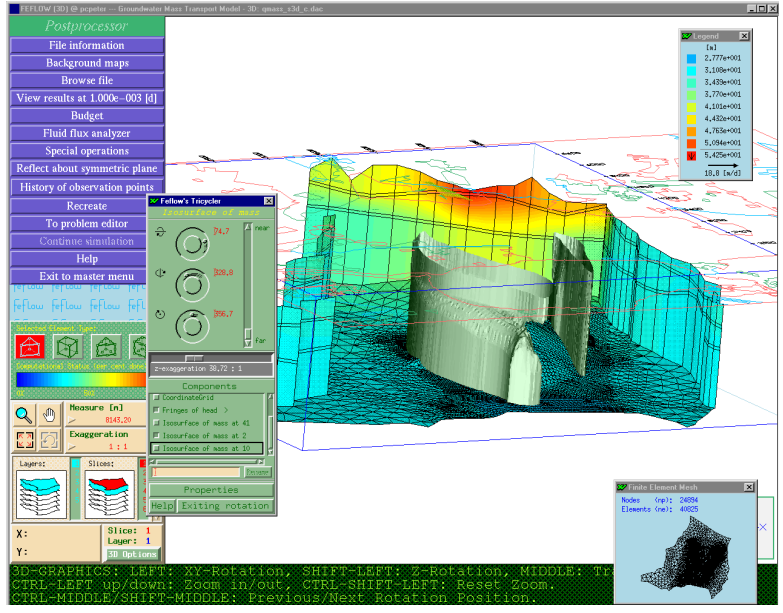
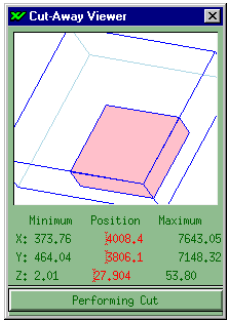


Figure 8.2 3D view.

8.4 Cut-Away Viewer



The **Cut-away viewer** defines the part of the projection to be cut away for an inside view of the parameter distribution. You can define the cut-out by inserting screen related **Position** coordinates in the menu or by moving the 3D handlers on the body of the model by mouse.

8.5 Pathlines Controller

The **Pathlines controller** pop-up menu lets you choose different modes of starting the pathlines, types of computation, shapes of the pathlines, and the number of pathlines to be visualized. It also allows to import starting points from a database (e.g., for computing the relevant area of influence around wells) and to export several 2D-projections of the pathlines.

Start by 3D cursor

To specify the starting point of the pathline drag the control handlers of the 3D cursor to the corresponding location of the model or enter the exact coordinates in the input text fields.

Start on 2D slice

Select between starting a single pathline or a number of pathlines specified in the input field along a line to draw or around a single well. The current slice field determines the slice at which the particles should start.

Relevant area of influence

This option allows the starting of multiple pathlines from a circle around a point at different elevations, e.g. at top and bottom of a well. You can either enter the point data manually or load a specific file (*.rai). See the online **Help** for a detailed description.

Use isochrone markers

Choose this option to enable the drawing of isochrone markers during the pathline computation. The set button opens a pop-up window for detailed isochrone settings (time levels, final time, and porosity/sorption values).

Foreward/backward

Isolines can be computed forward from the starting point or backward. Use backward, for example, to create pathlines starting from a well.

Options

Use this button to set the Pathline Outfit, the Numerical Parameters for the pathline computation and to choose between original and current stratigraphic data for the 'Start on 2D slice' option in case of moving meshes (Slice selection).

2D projections

The 3D pathlines can be projected onto a 2D plane after computation. You can select between different options:

- Horizontal plane for horizontal projections
- Vertical along pathline to create a vertical cross section which follows the pathline
- Vertical plane defined either interactively or by a segment

The exaggeration can be specified for vertical projections after displaying the projection. All 2D projections can be saved either in different graphics formats (Save picture as plot file) or as a point file (Save curves for diagram).

For detailed information see the Tutorial (Section 10.4.5) or invoke the context-sensitive online **Help**.

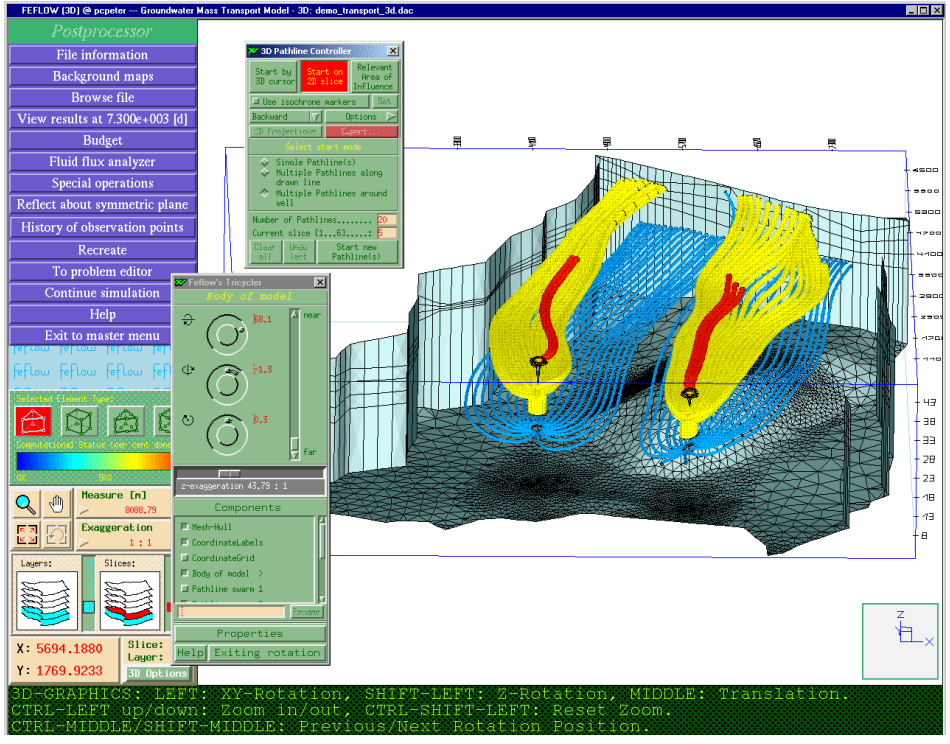


Figure 8.3 3D Pathlines controller.

FEFLOW Tools

9

9.1 FEPLOT

FEPLOT is a Windows-based plot tool for spatially related FEFLOW output, for ESRI shape files, and for AutoCAD *.dxf files. The handling of the program is mostly GIS-oriented. The import of OLE objects from other Windows applications in FEPLOT and vice versa is supported, as is the interface to the Windows print environment.

9.1.1 General settings

All objects of a current plot are listed in the object tree on the left of the working window. All toolbars as well as the object tree can be moved, resized or hidden.

The settings of the page size are defined in the Page setup option of the File menu. This option is available if you are working on an empty document or if you have loaded a template or a *.plt file.

The units of the page and map coordinates are set in the Preferences option of the File menu.

9.1.2 Objects

You can visualize and arrange several types of objects:

Map objects

Map objects may contain

- temporary plot files saved in FEFLOW (Windows only),
- map objects saved in the FEFLOW specific *.plx file format,
- shape files, and
- ASCII topology files (polygons, lines, points)

You can load several files on different layers in one map object, e.g., two different isoline contour maps of the same area. The plot object is organized in the Properties menu.

***Notice**: UNIX users should save the plots as plx files via the Capture option in FEFLOW or via the FEFLOW Data Store Manager. This file format is - like all FEFLOW export formats - compatible to the Windows environment.*

Draw objects

You can create lines, rectangles, rounded rectangles and ellipses in FEPLOT. The draw objects settings are specified in the Draw Properties menu.

***Notice**: All plots exported from FEFLOW use map units of meters.*

Text objects

Text objects are created in FEPLOT. The text objects settings are specified in the Text Properties menu.

OLE objects

Include other Windows-application objects in your FEPLOT plot compositions like spread sheet tables, diagrams or images. You can import these objects (active links) via the Insert new object option of the Edit menu.

9.1.3 Creating a plot composition

You can start a new plot composition by inserting map objects or by drawing objects on the default page using the options of the Draw menu. It may be more comfortable to load one of the predefined templates (.plt format) via the Open option of the File menu.

Templates contain the definition of

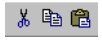
- page size,
- size, position and type of plot objects,
- size and position of other objects.

Save plot compositions in the FEPLOT specific *.plt file format.

Toolbar

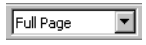
Most of the program handling can be done via the buttons in the toolbar:

Use these buttons to create a new plot, to open or save a plot composition.


The cut, copy and paste buttons work identically as in most other Windows applications. Using copy and paste the whole plot composition or a parts of it can be transferred to other Windows programs maintaining full quality, e.g., to save the plots as images using an imaging software or to include the plots into a report.

Hitting the delete button the currently selected objects are deleted from the plot composition.

The print section of the toolbar offers the possibility to open a print preview and to print the plot composition to the currently active printer.



Set the zoom factor for the working window using the zoom factor switch.

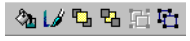
The help button invokes the FEPLOT online help system.

Having the arrow button activated, objects can be selected in the working window by mouse click. Press the <Shift> button to select several elements.

This section contains perhaps the most important buttons of the toolbar, from left to right:

- *New map frame*: Draw a frame with the mouse to contain a map object, such as a *.shp map or a *.dxf drawing. Each map frame can contain different maps in several layers.
- *New legend frame*: Draw a frame in the working window to contain a legend for a particular map frame. The button is only active if a map frame is selected.
- *New scale bar frame*: Draw a frame on screen for a scale bar related to a particular, already selected, map frame.
- *New north-arrow frame*: Draw a rectangle with the mouse to contain a north arrow. Direction and shape of the arrow can be specified later.

Use the text and drawing tools to add headers and frames to your plot composition.



The graphics tools provide functionality to fill polygons, to change line colors, to range the objects, and to group or ungroup objects.

Drawing properties

For each object a *Properties* window can be invoked by clicking the object with the right mouse button and selecting 'Properties' from the pop-up menu. In general, all properties of the object can be changed here, like color settings, positioning of the object, text style or shape and rotation angle of a north arrow. The most comprehensive properties window is that of a map object, which is described in detail below.

Drawing properties of a map object

The drawing properties window is organized in five different tabs:

Layers

In the Layers tab layers can be added or removed from a map object. A file loaded using 'Add' can contain one or several layers, depending on the file type. Use the 'Up' and 'Down' buttons to sort the layers. 'Info' displays some basic information about the layer. The 'Classify' button, which is enabled for maps containing attribute data, opens another window called 'Classify' to describe the classification of the layer based on attribute data. The classification is used for the coloring, e.g., for fringed maps or isoline drawings, and for the legend. See the detailed description of the classifying process below. With 'Layer title' a title can be specified different from the file name, which is set by default. The title is used for the legend. With 'hide layer' activated, the layer will not be drawn, neither on screen nor in printed output.

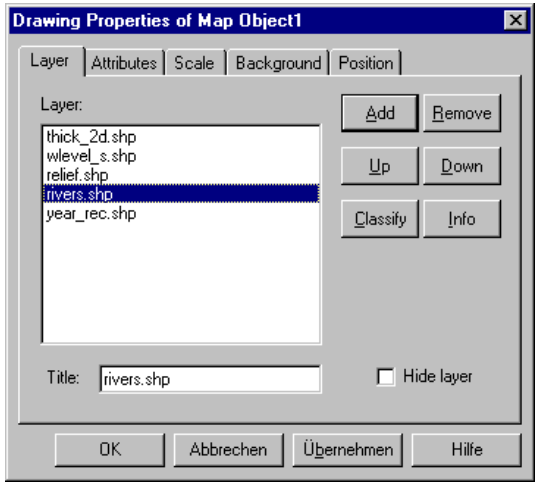


Figure 9.1 Drawing properties - Layers tab.

Attributes

The 'Attributes' tab provides functionality for editing the colors and display options of the different layers and the different classes of a layer. Choose the layer to edit using the 'Layer' switch. In the 'Identifiers' list below all available classes for the layer are shown. Selecting one or several classes, their properties can be set in the right part of the window ('Attribute' section). 'Feature' determines whether the settings below are used for the 'Outlines', the 'Foreground', the 'Background' or the 'Text' items. A line map does only contain outline information, while a polygon file contains outlines, and, if the polygons contain a hatched filling, a foreground color (hatch) and a background color. The color is set using the 'Color' switch. The 'Style' switch below determines the style, e.g., if lines are drawn solid or dashed, or if polygons are filled solid or hatched. 'Weight' is only active for the 'Outline' feature and

prescribes the line thickness. 'Title' lets you set a different title for the class, which is shown in the legend.

Scale

The scale can either be variable, so that it is changed when the size of the map object is changed, or it can be fixed to a prescribed value. The extent of the map object is either fit to the largest of the layers or to a specified layer. The x-y ratio can be set to 'fixed' or 'variable', too.

Background

The background settings determine shape and line width/filling of the map background.

Position

In the 'Position' tab the position of the map object on the page is specified.

Classify

Classification is a basic operation in geographical information systems (GIS). Attribute data for the different lines, points or polygons in the file is grouped to classes, which are displayed in different colors or with different styles.

For classification a column of the attribute data has to be selected using the 'Attribute' switch. In the lower part of the window four different options are available for the classification:

- *Single* creates one class containing all items.
- *Record* creates a class for each item.
- *Stage* creates a class for each different value appearing in the selected attribute column.
- *Range* divides the values in a prescribed number ('Classes') of equally spaced classes. For the attribute type 'Numeric' the minimum and maximum values can be chosen manually and the classification can be performed based on logarithmic data.

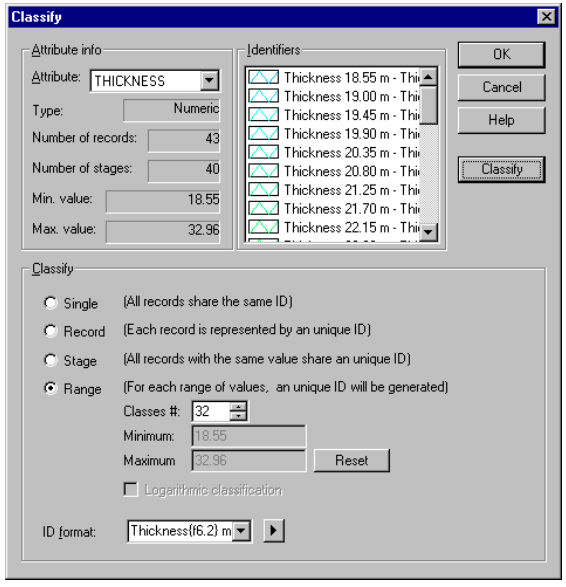


Figure 9.2 Classification window.

Additionally in the ID formats box the display format for the classes in the legend can be chosen. Hit the arrow shown at the right side of the ID formats box to select the numerical format. The format will be shown in the ID formats box between the braces in C programming style. This option is, of course, only available for the attribute type 'Numeric'. In the ID formats box itself a text can be added before or behind the braces, e.g, Head {f3.2}m leads to an output of 'Head 122.25 m - Head 123.25 m' for the class.

Hit 'Classify' to perform the classification. The resulting classes are shown in the 'Identifiers' list.

9.2 FE-LM²

9.2.1 What is FE-LM^2 and when is it useful?

The FEFLOW modeling system incorporates a number of constitutive relations such as saturation vs. pressure and hydraulic conductivity vs. saturation for unsaturated flow or absorption isotherms and reaction kinetics for reactive transport. Various parametric expressions are provided in FEFLOW to describe these constitutive relations. It remains for the user to select the best suitable expression and to identify the respective parameter set. The parameter-fitting tool FE-LM^2 was designed to assist in this task, typically known as 'curve-fitting.'

Built around a *Levenberg-Marquardt* Local Minimizer, FE-LM^2 provides instantaneous graphical feedback of a best fit when switching between parametric models and during user-controlled gradual changes in the weighting of selected data points. Possible local minima in the optimization function can be immediately recognized and subsequently circumvented by modifying the parameter ranges and optimization starting values through the user interface. As a parameter is gradually changed or explicitly set via the interface controls, the displayed shape of the corresponding model curve continuously tracks the user input.

Coupled models that share parameters can be fitted simultaneously to their respective data sets with graphical feedback provided for each set. The catalog of parametric models provided in FE-LM^2 includes all those implemented in FEFLOW.

9.2.2 Parameter estimation by residual minimization

The Levenberg-Marquardt algorithm minimizes a function q defined as the sum of weighted, squared residuals according to

$$q = \sum_i^N w_i(r_i^2), \qquad r_i = \frac{y_i - \hat{y}(x_i, \boldsymbol{p})}{\sigma_i}$$

where x_i, y_i, σ_i, r_i, and w_i are the measured independent and measured dependent variables, measurement standard deviation, residual, and weighting factor, respectively, at point 'i'. The total number of data points is N. The estimated dependent value is obtained from a **model function** $\hat{y}(x, \boldsymbol{p})$ utilizing the parameter vector $\boldsymbol{p}$.

Dividing the difference between measured and estimated dependent variable by the measurement standard deviation σ_i results in normalized, unitless residuals and makes q-values better suitable for comparison. Measurement standard-deviation values are either supplied by the user or will be estimated from the respective data set (see below). Weighting factors are included to permit data-point or data-set weighting that is unrelated to the certainty of the measured values, for example, to compensate for variations in measurement density within a set or for a difference in the number of data points between sets.

9.2.3 Data input file

FE-LM^2 expects at least one set of two-column (x, y) data where x is the independent variable. If a line contains more than two numbers, the third and/or fourth value will be read as an individual measurement standard deviation σ_i and/or squared-residual weight-

ing factor w_i for data point '*i*'. To distinguish a standard-deviation value from a weighting factor in the file, the latter must be preceded—without a space in between—by an asterisk ('*'). If both σ_i and w_i are given, the asterisk can be omitted. In this case, the four numbers on the line are taken to be in the order x_i, y_i, σ_i, and w_i.

While the standard-deviation values are considered as measurement-related and thus fixed, the weighting factors in the input file serve as initial values and can later be modified by the user via the FE-LM^2 interface to control the curve fit. Note that σ_i-values have the same units as the data while w_i-values are unitless.

The first line of a data set can be a set header containing the names of the independent and dependent variables, respectively, separated by at least one space. A name containing spaces must be enclosed in quotation marks, as in 'Time [min]'. Generic 'x' and 'y' labels will be assigned to all data sets for which no labels are given. One or two numeric value/s can follow (or replace) the two labels on the same line and will be interpreted as a measurement standard deviation and/or as a weighting factor (value preceded by a '*') that apply/applies to all data points in that set. Again, if both are given, the asterisk is optional unless there are no text labels present on the respective line. With no text present and both set-wide standard-deviation and weighting-factor values specified, the asterisk preceding the weighting factor is essential to distinguish the set header from a line containing an (*x*, *y*) data point.

Set-wide weighting factors permit inter-set weighting when fitting multiple data sets simultaneously. The default value for the set-wide weighting factor is 1.0. Individually specified w_i-values **are multiplied** with the respective set-wide value.

If no set-wide σ-value is given for a data set, an estimate will automatically be calculated using the measured values in the set as sample (this will thus likely be an overestimate):

$$\sigma\text{-}estimate = \left(\frac{1}{N_{Set} - 1} \sum_{i}^{N_{Set}} (y_i - \bar{y}_{Set})^2 \right)^{0,5}$$

where N_{Set} and $\bar{y}_{Set}$ denote the number of data points and the estimated mean of the measured values, respectively, in the data set. If the result is small enough to cause numerical difficulties or in case of single-value sets, the mean value of the set will be used as σ-estimate. Individually specified σ_i-values **take precedence** over the set-wide value.

Multiple sets have to be separated by either a label line or an empty line. The number of additional empty lines between data sets can be arbitrary.

In the example below FE-LM^2 recognizes two data sets. Values in the second set are believed to be more accurate which is expressed in a set-wide σ-value of 0.02 compared to that of the first set, 0.04. The first and second measurement in the first set are considered more reliable than the others in that set and are assigned individual σ_i-values of 0.01 and 0.02, respectively, while the last data point in the first set in considered less reliable with a σ_i-value of 0.07. All other points in the first set are assigned the set-wide value 0.04.

All points in the first set except for the last two are assigned the default weighting factor of 1.0. The last two data points in the first set are weighted by a factor of 2.0. To make up for the fewer data points, all points except the last one in the second set [ABC, XYZ] are weighted by a factor of 1.5. The last point in the second set is weighted by a factor of 4.5 (= 1.5*3).

```
'Pressure Head [cm]' Saturation
0.04
0 1.0 .01
-5 .98 .02
-10 .97
-25 .95
-50 .84
-100 .57
-150 .30
-200 .25
-300 .20 *2.
-500 .19 .07 *2.
ABC XYZ 0.02 *1.5
10 .735
20 .77
30 .795
40 .82
50 .845
80 .885 *3
```

Figure 9.3 Example data input file for FE-LM².

9.2.4 Loading the data set

A new optimization problem is created using the (Optimizer → New) menu entry or the associated toolbar button (). The user will be prompted for the name of the data file to be opened and for the selection of the data set(s) to be imported in case several sets are found in the file. Upon successful loading of the set(s), a ***Model selection and parameter control*** dialog will be opened for this optimization problem. For each set, the model providing the best fit when optimized from its default initial parameter values will be automatically selected among all implemented models and a new data-plot view window will be created.

Several optimization problems created in this manner can be open simultaneously. This can be useful to compare the fitting performance of different models for the same data.

The number of data sets within a particular optimization problem can be subsequently modified using the 'Import Data' and 'Close' commands accessible in the 'Optimizer' menu or via the associated toolbar buttons (and , respectively).

9.2.5 Control dialog

The ***Model selection and parameter control*** dialog shows a model selection box and value controls for all parameters of the currently selected model. Upper and lower bounds are shown for each parameter value and can be user-edited. The value of a parameter can be either edited directly or adjusted within the current bounds using the respective slider. Parameter values at their respective lower or upper bound are displayed in red.

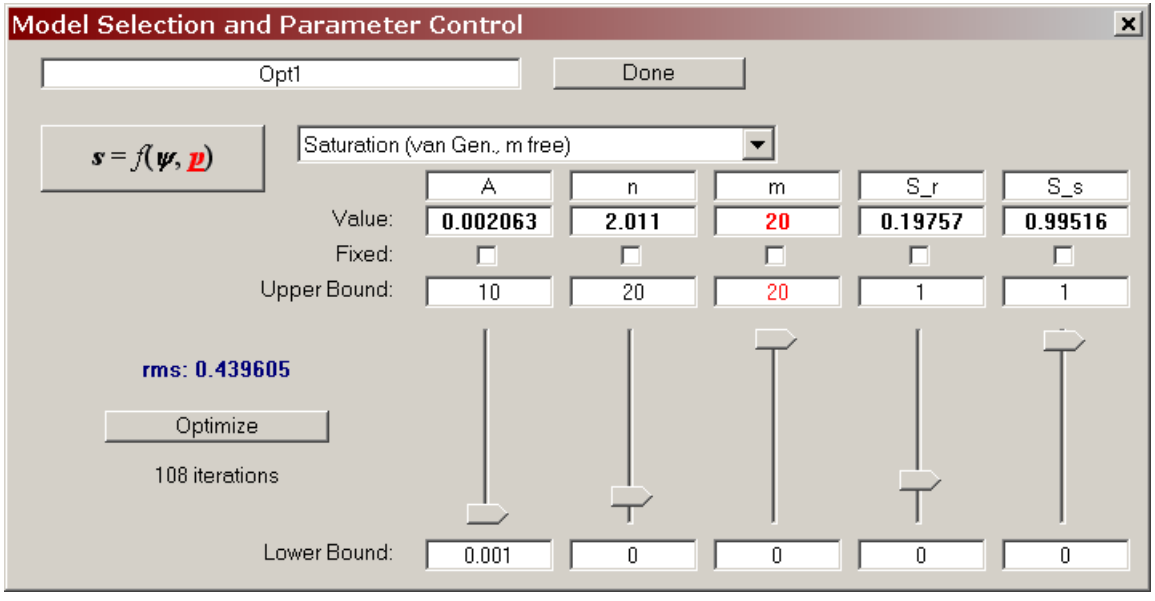


Figure 9.4 Control dialog for single data set.

As a measure of the current fit, the root of the mean squared residual (*rms*) is shown above the 'Optimize' button. Pushing the 'Optimize' button initiates a parameter optimization starting from the current parameter values. Parameters marked as 'Fixed' in their respective check box are not optimized. The number of iterations needed to converge at the local optimum will be displayed below the button.

The mathematical definition of the current fitting model can be displayed by pushing the model-equation button next to the model selection box in the dialog.

When multiple data sets are imported into a single optimization problem, the ***Model selection and parameter control*** dialog is extended so as to include a row of radio buttons for each parameter. The radio buttons are used to control parameter sharing between models.

Each selected radio button maps the parameter on the left in the button row to the value control at the bottom of the button row. Sharing is accomplished by mapping multiple parameters to the same value control. Each parameter is initially mapped to its own value control. For reference, the parameters mapped to a particular value control are highlighted while the respective slider is moved.

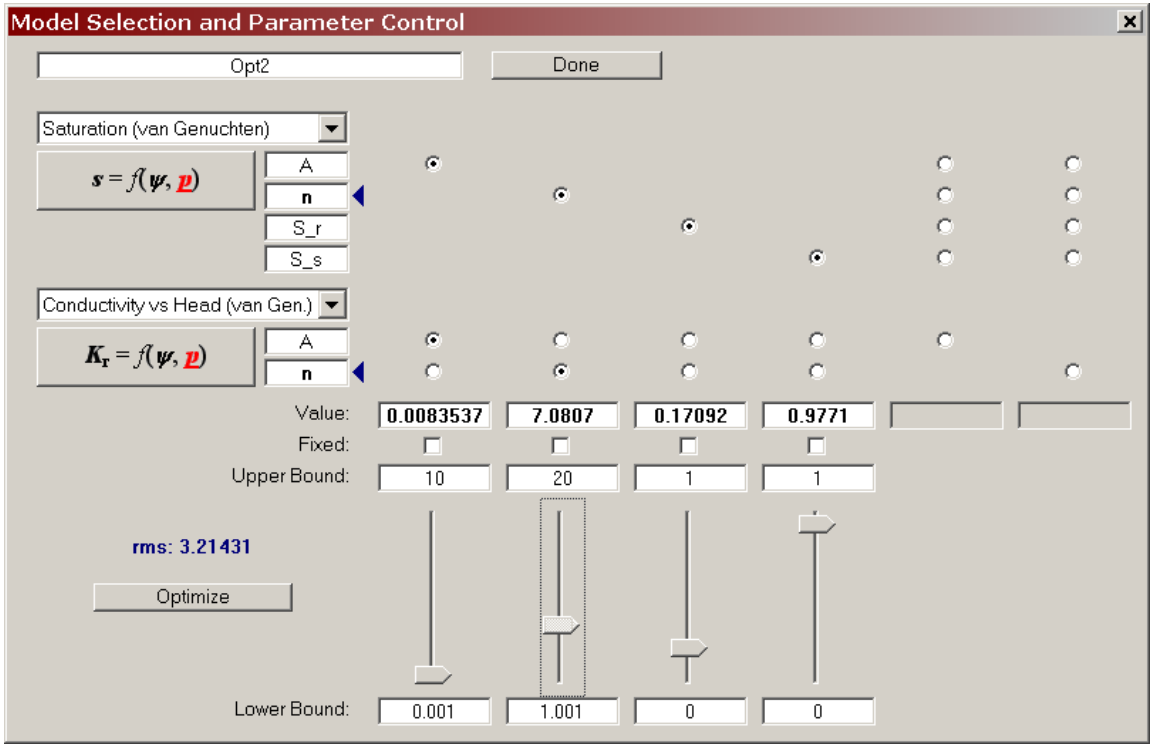


Figure 9.5 Control dialog for two data sets. Radio buttons have been set so as to share parameters '*A*' and '*n*' between both fitting models.

9.2.6 Data-plot view

The data-plot view initially shows all points of a data set together with a curve representing the best fit found by optimizing all implemented parametric models from their respective default initial parameter val-

ues.Thin horizontal bars are drawn one standard deviation above and below each data point. Thick horizontal bars are placed above and below each point at a distance corresponding to the respective standard deviation divided by the square root of the weighting factor; they will thus overlay the thin bars for all points that have a weighting factor of unity.

To toggle the displaying of error bars in the active data plot, use the 'Error Bars' command issued via the 'View → Error Bars' menu entry, via context menu (right-click in data-plot view), by pushing the associated toolbar button ( ), or by pressing the 'B' key.

When the cursor is placed over a data point, the values of the measured independent and dependent variable, of the standard deviation and of the weighting factor for that data point are displayed in the status bar at the bottom of the main window.

Data-plot views can be cloned (see below).

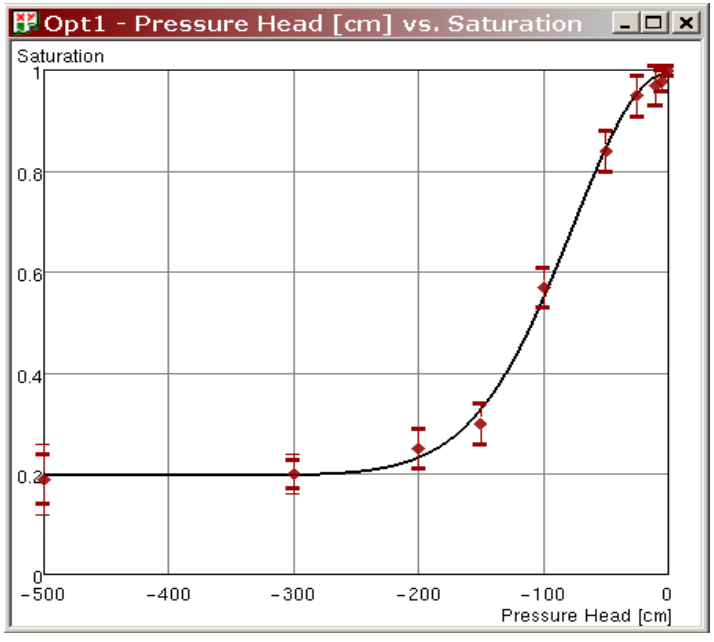


Figure 9.6 Data-plot view window.

9.2.7 Data-view cursor modes

Different cursor modes are available for a data-plot view window to provide the functionality to select data points and to navigate the plot. The cursor mode for the currently active data-plot view is set using either the respective entry in the 'Window → Cursor Mode' menu or the respective toolbar buttons. At any time, the cursor mode is one of the following five:

– *Selecting*
– *Unselecting*
– *Panning*
– *Zooming In*
– *Zooming Out*

The *Selecting* and *Unselecting* options are used to define a data-point selection to which weight modifications will be applied.

In *Panning* mode the data plot can be 'grabbed' with a left mouse-button click and moved within the plot window. Upon release of the mouse button, a new plot is constructed as close to the desired location as possible.

In either of the two *Zooming* modes, a target rubber box can be drawn with the left mouse button pressed. When released

- while zooming in, a new plot filling the data-view window is constructed from the area within the rubber box,
- while zooming out, the area of the entire current plot is collapsed into the rubber box area.

Temporary mode switching is activated by pressing and holding the 'Control' and/or 'Shift' key/s as follows:

- Pressing the 'Control' button while in *Selecting* or *Unselecting* mode will temporarily switch to *Zooming-In* mode. Pressing the 'Control' button while in *Zooming-In*, *Zooming-Out* or *Panning* mode will temporarily switch to *Selecting* mode.
- Pressing the 'Shift' button will temporarily switch the cursor mode between *Selecting* and *Unselecting*, and between *Zooming In* and *Zooming Out*.

Initially, the cursor mode is set to *Selecting*. Pressing the 'Escape' key while drawing a rubber box will cancel the action.

9.2.8 Selecting and unselecting data points for weight modification

Select and unselect

- Single data points by clicking on them while in the respective cursor mode,
- Groups of points by drawing an encompassing rubber box with the left mouse button pressed while in the respective cursor mode,
- All points using the respective context-menu (right-click in data plot) or 'Data' menu entry.

Note that any selected point remains selected until explicitly unselected.

9.2.9 Weight modification

Weighting factors of selected data points in the active plot window are modified using the ***Weight modification*** dialog. Once at least one data point has been selected in the active plot window, the dialog can be opened via the 'Data → Modify Weights' menu entry, via context menu (right-click in data plot), by pushing the associated toolbar button (), or by pressing the 'W' key.

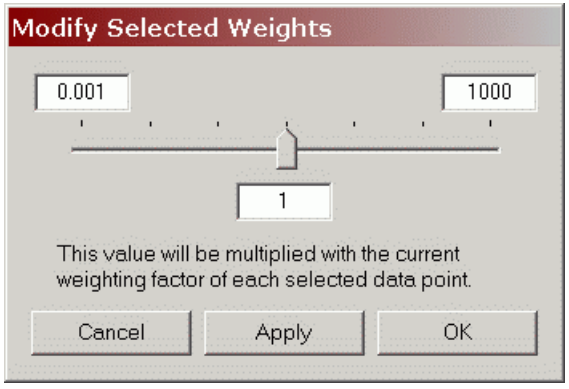


Figure 9.7 Weight-Modification Dialog.

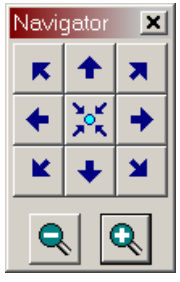
The upper and lower bounds for the modification factor can be user-edited. The value of the modification factor can be either edited directly or adjusted within the current bounds using the slider. The weight modification is dynamically applied to all selected data points; the point selection can be modified while the dialog is open. The effect of the current weight setting on the fitted model curve is instantaneously shown as optimization is performed automatically following each change in weighting.

The weighting factor of all selected data points in the active plot window can be explicitly set to unity with the 'Discard Weights' command issued via the 'Data → Discard Weights' menu entry, via context menu (right-click in data plot), by pressing the associated toolbar button (), or by pressing the '1' key.

9.2.10 Data-view navigation

There are several methods for navigation within a data plot:

- The 'Zooming' and 'Panning' cursor modes can be used as described in the Cursor-Modes section.
- To set the active data plot to its unzoomed initial location, use the 'Reset' command issued via the 'View ‡ Reset' menu entry, via context menu (right-click in data plot), by pushing the associated toolbar button (), or by pressing the 'Return' key. The arrow keys can be used for incremental panning in the direction of the respective arrow.
- In any cursor mode, the active data-plot can be panned with the pressed middle mouse button (or the pressed mouse wheel) and zoomed by turning the mouse wheel. Pressing the 'Escape' key while panning with the pressed middle mouse button will cancel the action.
- Push buttons for incremental zooming, incremental panning, and resetting of the data plot are provided in the ***Navigator*** dialog. The dialog can be opened via the 'View → Navigator' menu entry, by pushing the associated tool-



bar button (), or by pressing the 'N' key while a data-plot view is active.

9.2.11 Data-view cloning

Multiple plot-view windows for the same data set can be open simultaneously and navigated independently, e.g., to focus on certain portions of the set while also maintaining an overview of the entire plot. Multiple views for the same set are obtained by using the 'Clone' command on an active data-plot window. The command is issued via the 'Window → Clone' menu entry, via context menu (right-click in data plot), by pushing the associated toolbar button (), or by pressing the 'C' key.

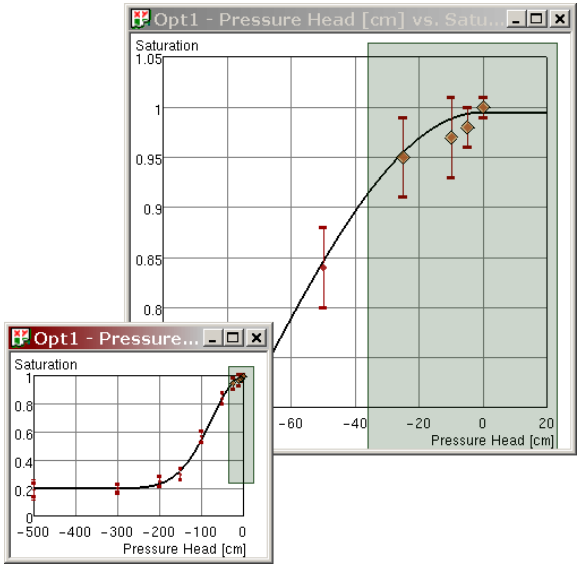


Figure 9.8 Data plot views associated with the same data set, shown with point-selection rubber box.

9.2.12 Exporting data fits

A fitted data set can be exported to a regular ASCII text file with the 'Export Fit' command issued via the 'Data → Export Fit' menu entry, via context menu (right-click in data plot), or by pressing the associated toolbar button ().

The exported file will contain

- Variable names and the name of the fitting model in a header line,
- Columns with measured independent and dependent values, measurement standard deviation, weighting factors, and model-predicted values,
- Parameter names and values.

Output files can be imported as data files for subsequent alternative fittings.

9. FEFLOW Tools

Part II

Tutorial

Tutorial

10

10.1 Introduction

10.1.1 Abstract

A two- and a three-dimensional flow and transport problem will be modeled in FEFLOW using realistic project data. All necessary steps are explained. Pre- and postprocessing of data is executed in FEPLOT and by using ArcView.

10.1.2 Scope and structure of the tutorial

This tutorial introduces the advanced user to the philosophy of modeling complex two- and three-dimensional flow and transport problems by using FEFLOW. It demonstrates the use of sophisticated functions and tools like time-varying boundary conditions and material parameters, complementary boundary constraints or grouped balance points.

First we will create a complete two-dimensional flow and transport problem based on realistic data. Afterwards we will extend the model to the third dimension.

For this exercise you need the **Tutorial** data on your harddisk. If the files have already been installed, they are located in the FEFLOW installation directory in a folder called **tutorial**. Otherwise you have to run the FEFLOW setup program again in **Modify** mode. Add the tutorial package additionally by checking the square besides the 'Tutorial' entry.

As it is not always easy to verbally describe actions to be done on screen we will make use of some signs. This may help in associating the written description with graphical information provided by FEFLOW. The signs illustrate various types of input:

- menu command
- button
- input field for text or numbers
- switch toggle
- radio button or checkbox

Please notice that the color of the corresponding element in FEFLOW may be different, depending on the window in which the element occurs. You will find for example green menus or yellow switch toggles as well as the blue ones shown above.

All file names are printed in color.

***Notice**: This tutorial does not include detailed instructions for the different input tools, options etc. We assume that you have gone through the Demonstration Exercise before and that you are familiar with the FEFLOW menu structure.*

10.2 Scenario

The spatial data described below are visualized as view in ArcView in the tutorial\gis\av3\directory

- win_start_demo.apr for Windows NT/95,
- start_demo.apr for UNIX.

You should define the environment variable wasydemo for the path "c:\program files\wasy\feflow 5.1\demo" before you load the *.apr file with ArcView (only for Windows).

Topography and land use:

The area under consideration is situated in the east of Friedrichshagen, a small town southeast of Berlin. The area is bounded in the south by lake Müggelsee, in the west by the river Friedrichshagener Mühlenfließ, and in the east by the river Neuenhagener Mühlenfließ. The northern boundary follows a groundwater contour line in east-west direction.

While the hilly northern part of the area is used mainly for agriculture, the plain southern part is covered by forest. Two towns are located in the study area: Friedrichshagen lies in the south-west, adjacent to the lake. Neuenhagen is situated in the north-east, bordering the forest and partly located above a waste-deposit site. An industrial area in the north-west includes a sewage treatment plant. In the south-east, near the lake, the city of Friedrichshagen has installed a well gallery consisting of four wells for pumping drinking water.

Geology/hydrogeology:

The geology of the area is characterized by quaternary sediments. The hilly area in the north is built up by outcropping glacial sediments, clays and overlaying sands. A flow channel filled with poorly sorted sand comes down from the north, dividing the area in two parts.

These structures are eroded and/or covered by alluvial and aeolian sands in the southern part of the area.

While the glacial clays are aquitards the top layer of sandy sediments with a thickness of up to 5 m can be characterized as a good unconfined aquifer. A second, lower, aquifer is situated below the clay sediments with a thickness of up to 30 meters.

10.2.1 The Task

For this fictitious scenario we assume that in 1988 an elevated concentration of nitrate has been detected in the drinking water of Friedrichshagen. Two of the four pumping wells became contaminated. The town accuses the sewage treatment plant as contaminator. The plant was built in 1971. Another possible source is seen in the Neuenhagen waste deposit, in use since 1974. We will simulate the spreading of contaminant mass from the two potential contamination sites, beginning in 1971, to help answer the following questions:

(1) Who is the most likely contaminator?

- plant, constructed in 1971, northwest of the wells
- waste deposit, in existence since 1974, northeast of the wells
- both
- neither

(2) Will the lake be contaminated?

(3) Has the peak contamination already passed or will concentration levels increase further?

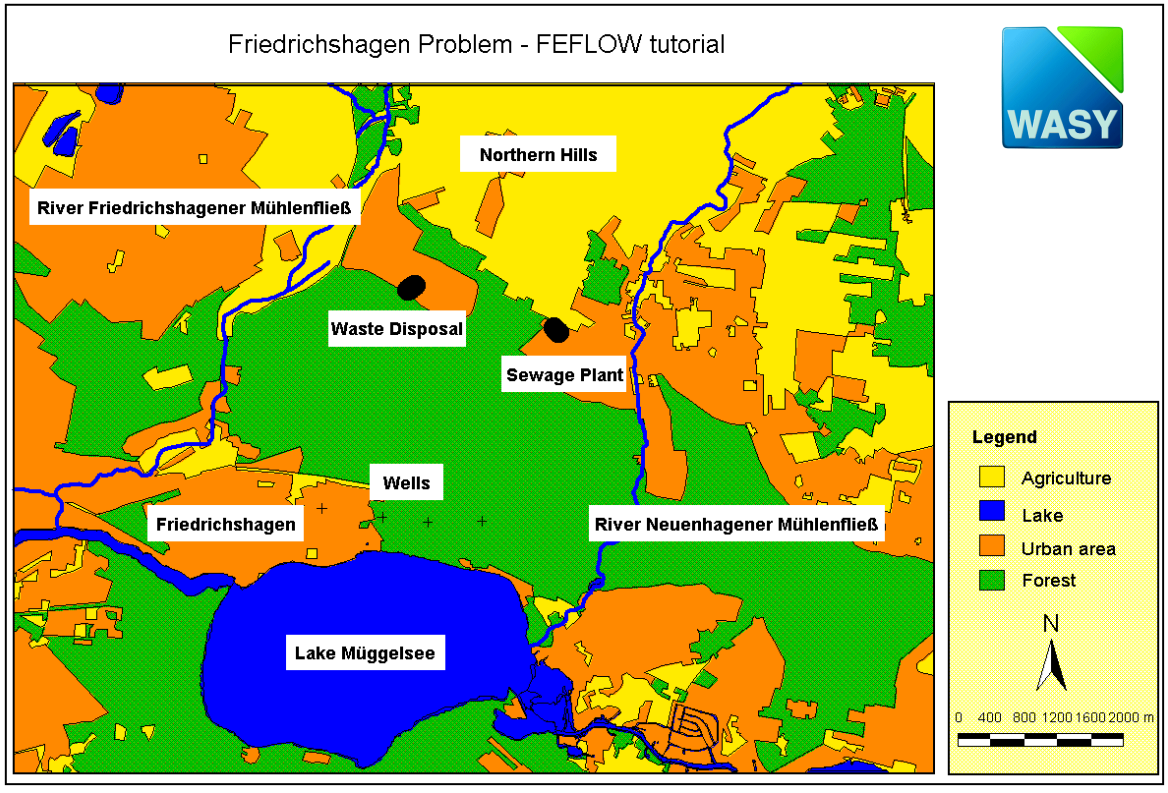


Figure 10.1 Overview of the modeling area.

10.3 The 2D Model

10.3.1 Step 1 - Basic structure

10.3.1.1 Designing the superelement mesh

__Notice__: Superelements cannot be subdivided. Drawing 'inner' superelements within an existing 'outer' superelement would result in an overlaying of the inner superelements over the outer one! Therefore, always create superelements side by side. If you design a superelement adjacent to an existing one, click on every node along the common sideline (highlighted if cursor is near) to ensure complete connection (unconnected parts will be treated as impervious).

The superelement mesh represents the basic structure of the study domain. The superelement mesh should be designed so as to take into account all locations where boundary conditions will be applied, or where the density of the finite-element mesh should vary. Be aware that the shape and the size of the generated elements can differ between outer and inner regions of a superelement, depending on the mesh-generator type used. As the rule, if a more homogeneous mesh is desired, graded and well-formed superelements should be preferred (see Figure 10.2).

First of all we have to decide what kind of finite elements we want to use. Open the **Options** menu of the shell and ensure that "**Mesh triangulation**" is selected. Triangulation has the advantage that you can create complex superelements containing as many border nodes as necessary. The resulting flexibility in mesh design is often important for real-world problems. Using mesh quadrangulation, a superelement cannot have more than four sides (this is enforced automatically by the Mesh editor).

All of the superelement mesh design is done in the **Mesh editor** which is entered via the **Edit** menu of the shell.

Next, background maps are loaded via the **Quick access** menu (**Add map...** or **Map manager...**), invoked by clicking the green colored part on the left side of the screen. The maps are used as templates for the mesh-creation process.

You will need the following maps:

- model_area.lin outer borders of the model area
- landuse.lin land use
- wells.shp location of the wells
- mass_source.lin sites of the contaminators

In the pop-up **Map measure** menu push the **Attach area** button only for model_area.lin, this will georeference and scale the working window to the study area.

Now enter the **Mesh editor** via the **Design superelement mesh...** command of the shell **Edit** menu. Construct the superelements with the mouse (**Continue polygon design**). The outer borders are outlined by the model_area.lin map showing the lakeside (S), the two rivers (W, E), and the groundwater contour line of 40 m (N). You can activate the map, by using the commands below the **Continue polygon design** button, to achieve an exact positioning of the superelements on the corresponding lines. Use the **Correct superelements** and **Erase superelements** options to improve the superelements as needed.

Try to create a mesh as regular as possible based on the landuse.lin and model_area.lin background maps. At each node of a superelement FEFLOW will also create a finite-element node. This may be helpful for the exact positioning of boundary conditions, but if you don't want to click on every corresponding point, there are also other possibilities to control the placing of mesh nodes later on.

An example for the resulting superelement mesh is stored as sm2.smh (for directory, see Table 10.11).

The superelement mesh can be saved separately using the **Quick access** menu. You thus have the data to generate several alternative finite-element meshes using the same superelement mesh. Furthermore, a superelement mesh can be reloaded as template for the

setting of the problem attributes as discussed further below.

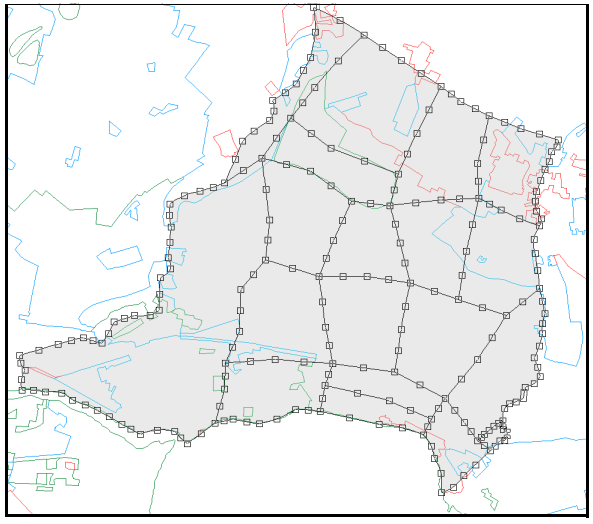


Figure 10.2 Superelement mesh.

10.3.1.2 Generating the finite element mesh

Enter the **Mesh generator** from the Mesh Editor menu (**Start mesh generator**) and select **Generate automatically**. A total element number of **500** is sufficient for our purpose. The resulting finite element mesh should look similar to the example file mesh2_1.fem (Figure 10.3).

We now want to refine parts of the finite element mesh. Enter the **Mesh geometry** menu. Select the **A-Join** tool and load the polygon file refine.ply as template for the area to be refined. The polygons have been designed in the **Reference data** section of the Problem Editor. As you can see in Figure 10.3, the polygons cover the area where we expect the contaminant to spread. Click on **Mesh enrichment** and select *Refine* from the small pop up menu. Now click on the polygons. See mesh2_2.fem for an example. Next, refine again the innermost polygons where the two potential contaminant sources and the pumping wells are situated.

We recommend to refine the area between the wells and the lakeside using the **Assign** - *Border* tool. The example mesh2_3.fem demonstrates how it could look after refinement. Afterwards, the middle polygons along the potential contaminant flow path have to be refined by **A-Join**. Finally, try **Assign** - *Single* to refine the area between the two flow paths.

Finish the meshing process by entering the **Check properties** menu. Compare the number of **Obtuse angled triangles** before and after executing the **Node movement by Laplacian operator**. The mesh should now look similar mesh2_4.fem (Figure 10.3) and contain more than 8000 triangles.

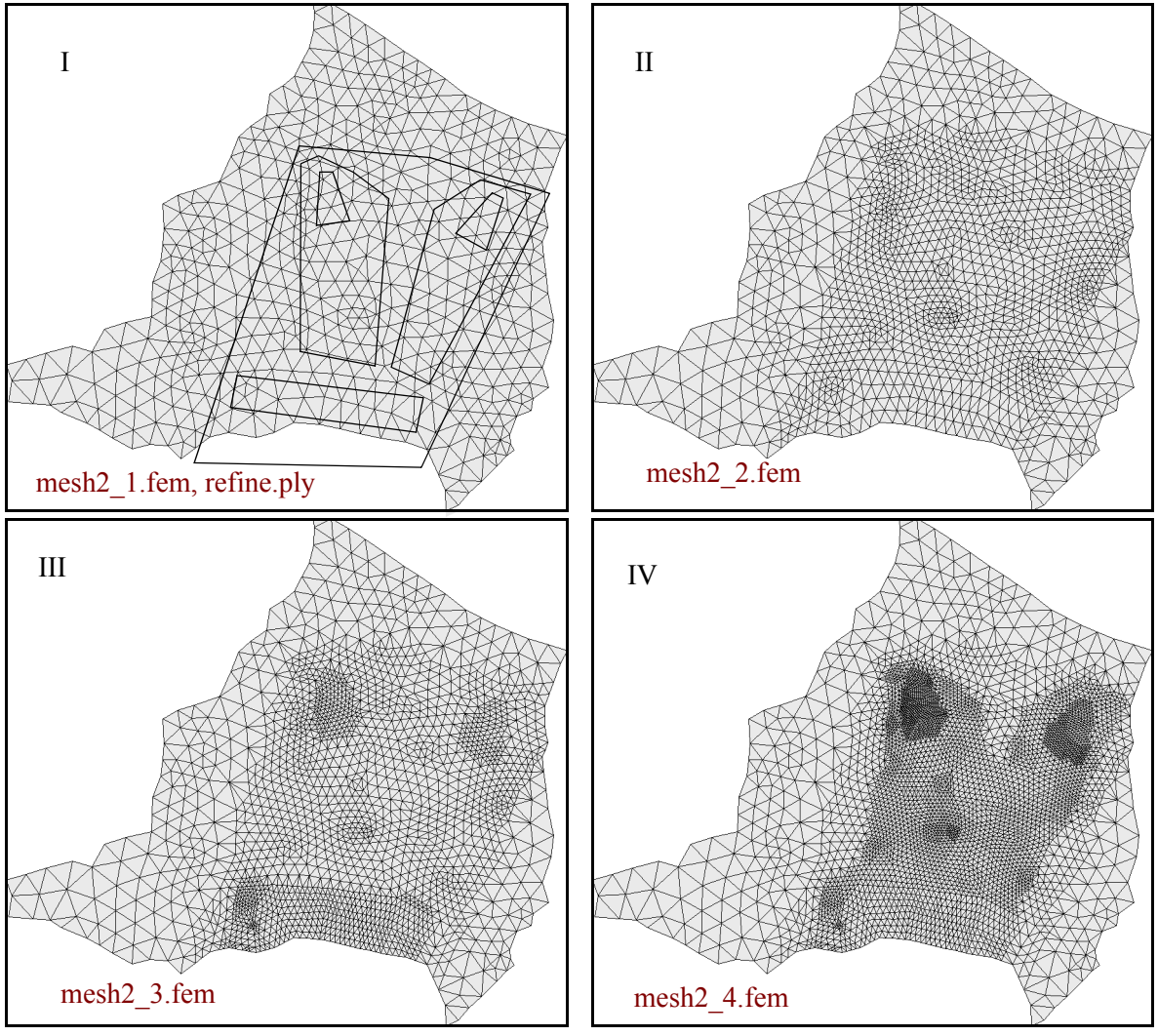


Figure 10.3 Refining the finite element mesh.

For the exact positioning of the contaminant-mass boundary conditions and for a realistic computation of the mass transport we refine the mesh at these locations.

- Select the **L-Join** tool and load the file mass_source.lin.
- Select **Mesh refinement** - *Refine*.
- Click on the highlighted lines in the mesh. The mesh is refined locally around the lines.

If it does not work, set a higher **snap distance**, i.e., define a wider area around the line to be refined, by clicking on the small blue **Snap** button next to the **Load** button of the Join options. An input box pops up. Insert a higher value (in pixels or reals).

10.3.2 Step 2 - Editing the problem parameters

To edit all problem-specific parameters, we now enter the **Problem editor** via the *Edit problem attributes* option of the **Edit** shell menu. A number of submenus has to be examined.

10.3.2.1 Problem class

In this menu you have to define the type of the simulation problem. First, we create a model for

- **Saturated media (groundwater)** as a
- **Flow-only problem** with
- **Steady flow conditions** and
- a **Confined** aquifer, using
- a **Horizontal** projection of the area.

We can safely ignore the time-step control parameters because we are simulating a steady-state flow.

10.3.2.2 Flow data

The parameters for saturated or unsaturated subsurface flow are set using the Flow-data menu.

Flow initials

Enter the Flow-initials menu and load the data via **Assign** - *Database* (**Akima** interpolation, linear, 3 neighbors, 0% over/undershooting) from the ASCII trp file head_ini.trp.

Flow boundaries

Enter the **Flow boundaries** menu to set the boundary conditions:

The northern boundary lies in the clay region, so not much water will enter the model domain from there. We will model an inflow of **-7.5e-02** m^2/d using the second-kind (Neumann) boundary condition.

Note the unit m^2/d and the negative sign. For a 2D horizontal confined model, no information about the thickness of the aquifer is required, so a parameter like the 2nd-kind boundary condition has to be considered as depth-integrated:

velocity [m/d] x thickness [m] =
depth integrated velocity [m^2/d].

Activate the Assign - *Border* tool and choose **Flux (2nd kind)**. See Figure 10.5 for the location of the boundary conditions.

The rivers will be described by a third-kind (Cauchy) boundary condition, **Transfer**. For this kind of boundary condition you have to define a spatially variable *Reference Hydraulic Head* in the flow-boundaries menu, describing the water table in the river. The flow between this surface water and the groundwater body is must pass through a colmation layer, which will be modeled by assigning a **Transfer rate** in the

***Notice**: This step is recommended in order to test the suitability of the mesh and the quality of the flow parameters. Even if the real hydraulic regime is unconfined it is useful to test the model under confined conditions first because the computational effort is smaller and therefore the simulation is much faster.*

***Notice**: Check the coordinate system before the interpolation in the lower left corner of the screen. The setting should be "global".*

***Notice**: For flux boundary conditions inflows are negative, outflows are positive!*

Flow materials menu later on (see Reference Manual, Section 4.2).

Use the Join tool with the Data option and load rivers.lin.

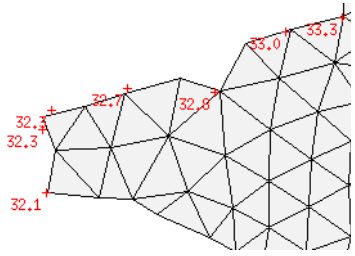


Figure 10.4 Regionalization.

Click Transfer, choose 1 D linear interpolation along lines, and import the time constant data from the file wlevel_w.trp. Click Apply to perform the regionalization. Choose Interactive selection lines for joining, click Okay and click on the lines along the western border. Repeat the steps above for the eastern border by importing the file wlevel_e.trp.

Now we have to define the lakeside boundary conditions in the south. We recommend to use the **Head (1st kind)** boundary condition with a hydraulic head of **32** m which has to be **Assigned** on every *Border* node.

The positions of the wells and pumping rates will be imported from a file mean_well_rate.trp with the *Database* option of the **Assign** tool as 4th-kind boundary condition, **Well**.

Perform the regionalization by Inverse distance weighting interpolation (1 neighbor, Import time-constant data).

Click on **Apply**.

Select **Well (4th kind)** from the menu, choose 'Interactive' in the pop-up alert box, and hit the <F2> key. FEFLOW executes an automatic mesh refinement with an exact positioning of the four wells ('Mesh nesting').

You can check the input data by using the **Mesh inspector** after clicking on the corresponding icon. If an outer or inner border node remains without explicit boundary condition, it will be treated as impervious to flow entering or leaving the model domain.

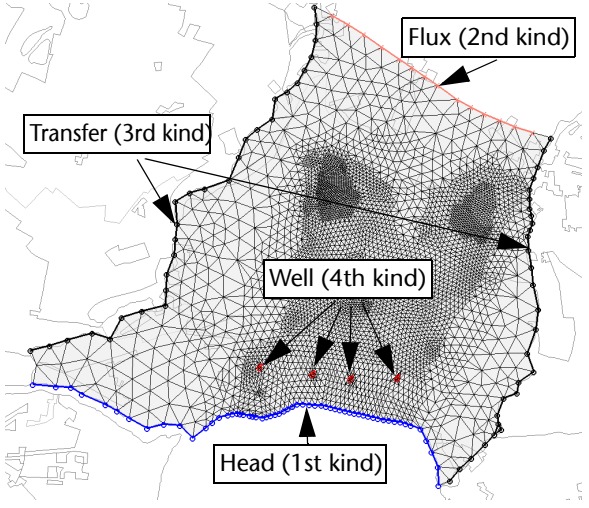


Figure 10.5 Model area with flow boundary conditions.

Finally, we create a background map of the locations of the wells. We will need it later in the **Reference** section.

Select the **Export** tool from the light blue button below the mesh inspector.

Click on the **Well (4th kind)** button. The **Exporting menu** pops up.

Export the locations of the wells as **Generate(2D)** file.

Leave the Flow boundaries menu now (**Return**) and enter the **Flow materials** menu.

Flow materials

Only **Transmissivity**, **Source(+)/sink(-)** for groundwater recharge, and the **Transfer rate** have to be defined. The values of transmissivity are the product of the conductivity multiplied by the local aquifer thickness. The aquifer thickness represents the summed thickness of the upper and the lower aquifer, the aquiclude is neglected in 2D. Load the values for **Transmissivity** from the corresponding triplets file via the **Assign** - *Database* tool:

trans_2d.trp (linear **Akima**, 3 neighbors, 0% over/undershooting, Import time-constant data).

For assigning the groundwater recharge to the "**Source(+)/sink(-)**" parameter we will use a polygon file as template and link it with a database:

Select the **Join** tool from the scroll list below the Mesh inspector icon.

Choose **Polygons** from the small Join-menu.

Now click on *Load*. In the file-selection dialog select the polygon file mean_recharge.ply.

Next, the database-selection dialog pops up. Select the ASCII Table mean_recharge.dat (if linking already exists this step is skipped).

The links between the polygon file and the database are edited in the **Item-database associator** popping up next. On the left-hand side the **Database items** list shows the field names of the linked database. On the right-hand side the **FEFLOW parameters** are listed. First you should define which database field contains the IDs of the polygons.

Click on **IDD** in the *Database Items* list, highlighting it.

Click on **ID** on top of the *FEFLOW Parameter* list.

Click on the **Add link** button on the right. The link is visually displayed.

Create a link between the database item **Recharge** and the FEFLOW parameter **Source/sink for flow** in the same way. You have to scroll the *FEFLOW Parameter* list by using the vertical slider bar for visualizing the source/sink for flow parameter. An additional field at the bottom of the menu allows to define optional conversion factors for the data transfer, which is not necessary for our data. The result of the linking should look like Figure 10.6.

Now click on the "Okay" button to leave the menu.

Click on the **Source(+)/sink(-)** button in order to activate the joining. A red alert box pops up asking you if you want to import the data for interactively selected polygons or perform automatic overlay.

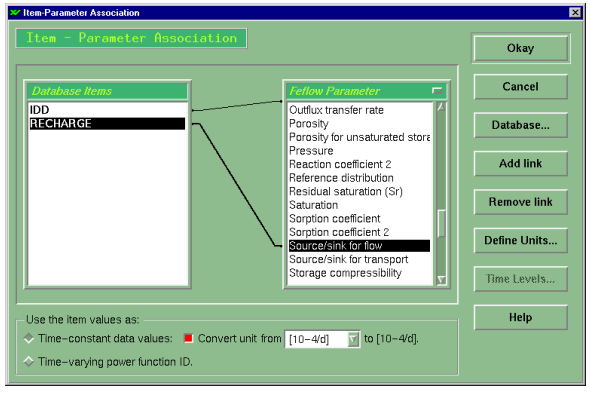


Figure 10.6 Item - Parameter Association

Click on the **Overlay** button. The Joining is executed automatically for all elements. You can visualize the values by using the **Show** tool.

Finally, we **Assign** *Global* values for the **Transfer rate**, assuming a colmation layer of approx. 1 m thickness and a K_0^{in} of 1.2e-05 m/s. For additional information about the Transfer boundary condition see

the Reference Manual, Section 4.2.

- Bu Transfer rate **In**: 10000 [1e-04 m/d]
- Bu Transfer rate **Out**: 40000 [1e-04 m/d] (typically higher than for inflow)

Leave the **Flow data** menu now.

10.3.2.3 Reference data

During the simulation FEFLOW will automatically display curves for hydraulic head at all wells and for the average mass concentration at flux boundaries and wells. To observe other points of interest, too, we have to provide reference-data information, i.e., we have to define observation points and observation-point groups.

Enter the Bu **Reference data** menu. Select Bu **Observation single points** and click on Bu **Set arbitrarily** for assigning points along the expected contaminant flow path. See Figure 10.7 for suggested reference-point locations. Alternatively, you can Bu **Import points** from the point file obs_pnts.pnt.

Now leave the **Single observation points** menu. For calculating the mass and flow balances for inner and outer boundaries at single locations or along sections (e.g. wells or rivers) it is useful to set Bu **Observation point groups**. Enter the corresponding menu and set five different point groups, one point as separate 'point group' on every well and one point group for the nodes along the southern (lakeside) boundary. You can use the background map of the well boundary conditions for **Point-joining** now. You have created this map earlier from the Flow boundaries menu.

For each point group you have to select a different ID from the **Group identifier** list first. Their mass and flow balances will be drawn in a special window during the simulation run. Return to the main menu of the Reference Data Editor.

For many analyzing techniques of FEFLOW the definition of fences or sections is useful. In the Bu **Fences (sections)** menu draw one line along the northern boundary, another from the North to the South dividing the model in two equal parts and finally north of the well gallery a line from west to east.

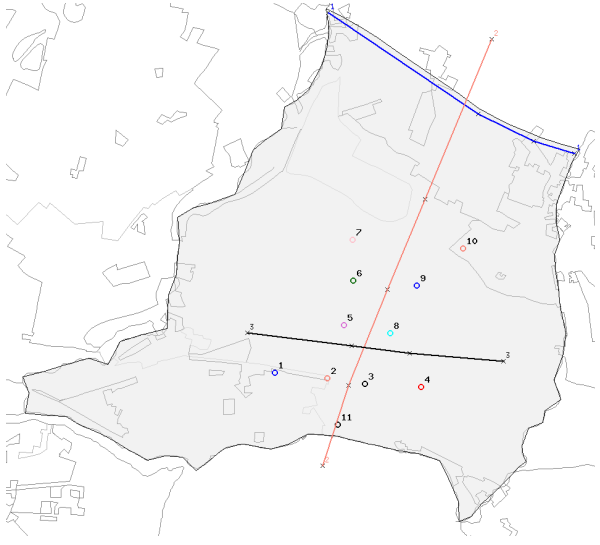


Figure 10.7 Fences (sections).

These points and lines become part of the finite-element problem file and can be selected in many menus via their IDs (displayed as numbers at the ends of the segments).

All required data have now been assigned now. **Before starting the simulation run save your finite element problem**, because the distribution of hydraulic head will - necessarily - change during the simula-

tion run. That means, the initial conditions will be replaced by the new time-level results. You can save the file via the **Quick access menu** or via the shell menu **File** (default file extension is *.fem). Saving is possible either in a binary file format, which is faster in writing and reading, or in ASCII file format, which can be read and even edited using any text editor.

10.3.3 Step 3 - Let's test it

10.3.3.1 Running the simulator

Leave the Problem Editor and enter the **Simulator** menu (**Run** - **Start simulator**). As a first test, we only want to see whether our mesh is designed well and if our input data for the hydraulic parameters give realistic results. We start the simulator by clicking on the **(Re-) Run simulator** command.

10.3.3.2 Halt and view results

After the simulation has finished, activate the **Results viewer** by clicking on **Halt & view results**, and select *Particle tracking*. Try the different items available in the **Options** submenu. Check the velocity field. If the pathlines suggest that there are impermeable sections in the model you likely made a mistake in designing the superelements.

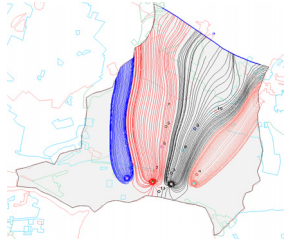


Figure 10.8 Particle tracking.

Activate one of the line segments you have created in **Line sections & segments** and display diagrams for the hydraulic head distribution. Leave the **Halt & view results** menu and select the **Budget** menu. Calculate a flow balance for the whole area. Check whether the values are realistic. The total imbalance should be approximately zero for this steady-state simulation.

10.3.4 Step 4 - Back to the problem editor and run again

Leave the simulator and load either your own *.fem file or the prepared file qflux_s2d_c.fem to retrieve the initial values. Re-enter the **Problem editor**. If the simulation run shows that our flow-only model works well we can now extend it to a flow-and-mass-transport problem. First, we redefine the problem class accordingly.

10.3.4.1 Problem class

Change the Problem Class to

- **Flow and mass transport**,
- **Transient flow/transient transport** for an
- **Unconfined** aquifer

and leave the **Problem class** menu.

10.3.4.2 Temporal & control data

In this menu we will set the parameters for the time stepping procedure during the simulation run and define the time-varying functions for flow and transport parameters to be assigned to the model:

Set the toggle for **Automatic time step control**, define an **Initial time step** of **0.001** d and a **Final time** of **7300** d.

To import and edit point-related time-varying data click the **Edit time-varying power functions** button. The **Power-function editor** window appears where time-related functions can be interactively edited. The so-called *Power functions* are (x, y) value pairs, where the x-values describe the time in days while the y-values define the corresponding function value. For example time-varying functions are applied to pumping rates or time-varying water levels in rivers or lakes. As soon as functions are introduced and actually assigned to the problem conditions, the function values will be saved within the finite-element problem file (*.fem). Having been created in this editor, the curve data can then be assigned in the **Flow data** and **Transport data** menus.

We will use the following items:

ID access

In this list all IDs of the power functions are displayed. Initially, all IDs are empty.

Import curve data

A file can be selected which contains function data in ASCII format to be assigned to the current ID. The correct syntax for files containing power functions is described in the **File-format library** of the online **Help**. A power function for curve data has to contain two columns, separated by empty space or tabs (t [d] fvalue [-]).

Load the power functions for the pumping rates of the wells by using the *Import curve data* button:

well_rates.pow

as a simple ASCII format file.

You can plot the values by selecting the ID in the **ID access** list. The curve is displayed as a diagram. Click on **Edit data list** for editing the value pairs.

Now, we leave the **Temporal & control data** menu and enter the **Flow data** editors.

10.3.4.3 Flow data

Flow boundaries

Taking into account the fact that the aquifer is unconfined we change the flux boundary condition to a depth-integrated boundary condition type. That means we will have a constant discharge of groundwater independent of aquifer thickness, which may change with the moving water level. Select **Options** in the tools list (below the mesh inspector icon), the boundary condition type **Flux (2nd kind),** and **Constant flux area** from the appearing submenu, and assign a value of

- 0,05 m²/d

along the northern border. The symbols for flux boundary conditions should be displayed with an additional integral sign.

We have to replace time-constant by time-varying boundaries with some constraints:

The four wells will get time-varying pumping rates. Activate the Assign - *Database* option using the same settings as before (Akima, linear, 3 neighbors, 0% over-/undershooting). This time import the file well_time_funcs.trp via the **Import power ID database** option from the lower right button

group. Start the regionalization, click on **Well (4th kind),** choose 'interactive', and hit <F2>. The time-varying boundary conditions are set. You can check the settings with the help of the Mesh inspector (zoom in first to locate the node of the well exactly).

As the screens of the wells do not reach to the aquifer bottom we have to set a **potential constraint** ensuring that well drawdown is limited to the depth of the lower end of the respective well screen. Conversely, a rising water table must not get too close to the ground surface. We thus have to set both a **minimum** and a **maximum potential constraint** for each well (zooming in as needed):

Table 10.1 Constraints for well BCs

Well ID	Min. [m]	Max. [m]
1	31.8	33
2	13	33
3	13	33
4	13	33

Click on the **arrow** at the right of the Well (4th kind) button. The corresponding **Constraint conditions** menu becomes visible.

Input the Min and Max constraints and click on the small toggles left of the input fields to activate the settings. Click on **Well (4th kind)** and assign the constraint to the corresponding well on the mesh (Table 10.1).

Repeat the steps for all wells.

Leave the **Constraints** menu via the **arrow** button.

Check the input by activating the Mesh inspector. If a constraint is set on a well the message 'time constant constraint behind!' is displayed in the inspector window.

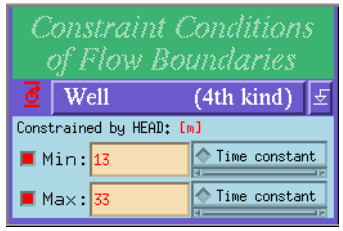


Figure 10.9 Constraint conditions.

Flow materials

The items of the **Flow materials** menu have changed with the problem class. Assign **Conductivity** and **Aquifer top- and bottom elevation** by importing and regionalizing the corresponding data via the **Assign** - *Database* tool (Akima interpolation, linear, 0% over-/undershooting, import time-constant data):

- conduc_2d.trp conductivity
- relief.trp aquifer top elevation
- bot_san2.trp aquifer bottom elevation

The groundwater recharge varies over time. The setting of the values is therefore a little different than before: We want to import the values directly from a database. We will use a polygon file as template and link it with a database which contains the groundwater recharge values for different times.

Select the **Join** tool from the scroll list below the mesh inspector icon,

Choose **Polygon** from the small Join menu.

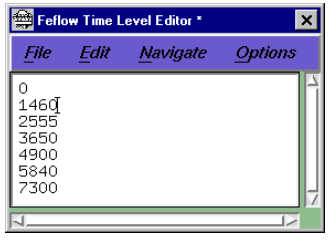
Now click on *Load*. In the file-selection dialog select the polygon file time_recharge.ply.

Now the database selection dialog pops up. Select the ASCII database time_recharge.dat.

The links between the polygon file and the database are edited in the **Item-database associator** that appears next.

Switch the list definition for the right hand list from **FEFLOW parameter** to **Time levels.**

Click on the **Time levels...** button on the right side. An editor pops up.



Insert the time stages in days for which different groundwater recharge distributions exist as shown in the image on the left.

Close the editor and confirm your input by clicking on the **Yes** button in the alert box. The time stages are shown in the **Time levels** list now.

The time levels have to be linked to the database items. As before, each polygon gets one particular value for each time stage. The polygons are identified by their IDs.

Let us define the database items which contain the IDs of the polygons.

Click on **ID** in the *Database Items* list, highlighting it.

Click on **ID** on top of the *Time Levels* list.

Click on the **Add link** button on the right. The link is visually displayed.

Continue to link all time levels with a database item according to the list below. Note that you can link the same database item with different time stages.

Now click on the “Okay” button to leave the menu.

Table 10.2 Linking of recharge values and time levels

Database item	Time Level
ULTRA_DRY	4900
DRY	1460, 7300
MEAN	0 5840
WET	3650
ULTRA_WET	2555

Click on the **Source(+)/Sink(-)** button to activate the joining. A red alert box pops up asking if you want to import the data for interactively selected polygons or by automatic overlay. Click on the **Overlay** button. The joining is performed for all elements.

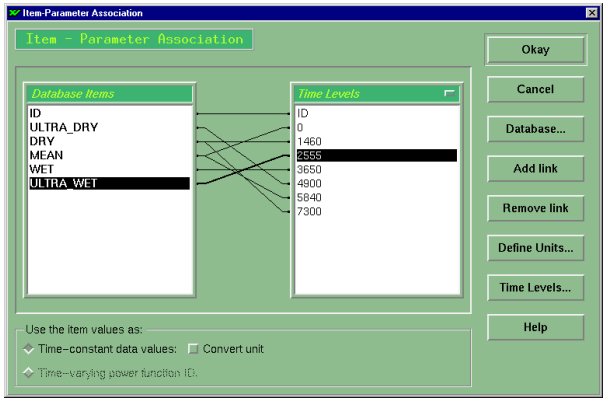


Figure 10.10 Linking of time levels and database items.

For copying and visualizing the time-varying data select the T-List tool and click on **Source (+)/**

Sink(-). The **T-List menu** pops up. You can control the time-varying curve for any place on the mesh by selecting **Preview defined time dependency**.

Move the two slider bars on the right and at the bottom of the model graphic in order to position the cross hairs on the element of interest. All Flow Materials settings are listed in Table 10.3.

Table 10.3 Material properties

Item	Unit	Default	Setting	Input type
Conductivity [Kmax]	$10^{-4} ms^{-1}$	1	conduc_2d.trp	Assign-database
Anisotropy factor	1	1	default	
Angle from +x-axis to Kmax	° degree	0	default	
Aquifer bottom elevation	m	0	bot_sand_2.trp	Assign-database
Aquifer top elevation	m	1	relief.trp	Assign-database
Storativity (drain/fillable)	1	0.2	default	
Storage compressibility	m^{-1}	10^{-4}	default	
Source(+)/Sink(-)	$10^{-4} md^{-1}$	0	time_recharge.ply time_recharge.dat	Join, polygon, Const.
In-transfer rate	$10^{-4} d^{-1}$	0	10000	Assign-global
Out-transfer rate	$10^{-4} d^{-1}$	0	40000	Assign-global

10.3.4.4 Transport data

The **Mass-transport initials** remain on the default value of 0 mg/l.

Mass transport boundaries

Time-constant boundary conditions:

In the **Mass-transport boundaries** menu the two contaminant sources have to be defined. After setting the **Join** tool for joining via *Lines,* push the *Load* button of the Join menu to load the file mass_source.lin. A database-selection dialog pops up asking for a database table. Click on ***Cancel*** in order to import only the geometrical data. The nodes to be covered by mass-transport boundaries are then displayed. Select **Mass**, enter a value of **50 mg/l** in the **Keyboard request box**, hit the <Enter> key and click on the line at the sewage plant (western contamination site) for assigning the time-constant boundary conditions.

Time-varying boundary conditions:

We do not want to ignore the fact that the waste-deposit site (eastern contaminant site) started its operation three years after the sewage plant. As the sewage plant is active during the whole simulation time we can keep the corresponding boundary condition time-constant. However, we have to assign a time-varying mass boundary condition for the deposit site.

Click on **Time-varying function IDs.** The **Power-function editor** pops up.

Click on **New ID** above the scroll list. A new empty power function is created. You can provide a short comment for the function in the **Comment line**, e.g., „waste massbc“. This is useful if many time-varying functions are created which cannot be identified easily by their IDs.

***Notice**: Constraint and boundary conditions are handled differently for fluxes:*

For constraint conditions inflows are positive (+), outflows are negative (-).

For boundary conditions inflows are negative (-), outflows are positive (+).

Click on **Edit time list** and type the lines of Table 10.4 in the appearing editor.

Table 10.4 Power function values

time	fvalue
0	0
1095	0
1095.1	50

Click on **Okay** to return to the **Mass-transport boundaries** menu and assign the time-varying boundaries at the waste-deposit site using the corresponding power function ID 5. Note that the toggle below the **Time-varying function IDs** button has been set automatically from *Time constant* to *ID* of 5, allowing to assign the ID in the same way as a time-constant value.

Constraints

The procedure is similar to the setting of potential constraints for flow boundaries. The only exception is here that two different types of constraints can be assigned: The first one can be described as complementary constraint, similar to the flow boundaries. The other type is the setting of Min. and Max. values for the hydraulic head. Only in the range defined by these values will the contaminant mass boundary be active. We will set a minimum value for the sewage plant to make sure that the contamination only becomes active if the aquifer is wetted. See the online **Help** for more details. Additionally, we set a mass boundary condition with the small value of 1e-12 [mg/l] along the whole outer border of the area together with a complementary minimum constraint of 0 [m³/d mg/l]. This so-called **Freshwater condition** ensures that the first-kind boundary

condition of fresh water is only set for water entering the domain at the boundary (inflow). For outflow, the first-kind boundary condition (fresh water) is automatically switched off and the contaminant mass can freely flow out (if the boundary is open for advection). For background information see the Reference Manual (Section 4.3).

Table 10.5 Mass transport boundaries and constraints

Place	Boundary condition	Complementary constraint	Additional constraint
sewage plant	Mass, first kind 50 mg/l	Min: -- Max: --	Min: 34 m Max: --
waste deposit	Mass, first kind Power ID 5	Min: -- Max: --	
outer borders	Mass, first kind 1e-12 mg/l	Min: 0 Max: --	

Transport materials

The items, **Porosity,** **Sorption coefficient and** **Longitudinal/transversal dispersivity** should be assigned via **Assign -** **Global**.

After having saved the *.fem file we return to the **Simulator** menu.

Table 10.6 Transport materials

Item	Unit	Default	Setting	Input type
Porosity	1	0.3	0.2	Assign-global
Henry-Sorption:				
Sorption coefficient	1	0	0.04	Assign-global
Molecular diffusion	$10^{-9} m^2 s^{-1}$	1	default	--
Longitudinal dispersivity	m	5	50	Assign-global
Transverse dispersivity	m	0.5	5	Assign-global
Decay rate	$10^{-4} s^{-1}$	0	default	--
Source(+)/Sink(-)	$\frac{mg}{l} md^{-1}$	0	default	--
In-transfer rate	$m^2 d^{-1}$	0	default	--
Out-transfer rate	$m^2 d^{-1}$	0	default	--

10.3.4.5 Simulator

Enter the **Control output** menu (see Figure 10.11) and define a *Complete Results* (*.dac) file in the file selector. A *Complete Results* file saves all data of the finite element problem, such as hydraulic heads, velocities and mass concentrations at each node and for each time stage. We want to save the results of every fifth step. The display output should be set to the same value in order to reduce the graphical effort during the simulation run.

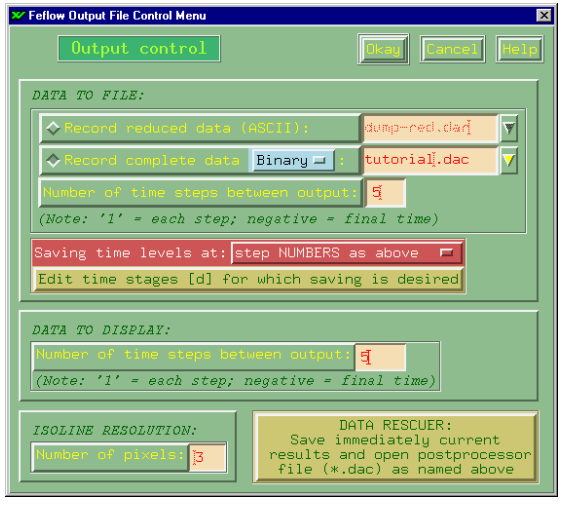


Figure 10.11 Control output window.

10.3.5 Step 5 - Analyzing the results

10.3.5.1 The postprocessor

The postprocessor provides various tools for analyzing and exporting computational results from a simulation session. It also allows to re-create a finite-element problem, or to continue an interrupted simulation run.

For entering the postprocessor, click on the corresponding menu item and select **Load and run...** Load either the .dac file created during the simulation run or the prepared file qmass_t2du.dac.

The **File information** option displays a table with information about the loaded model and the numerical characteristics used during the simulation.

In loading the postprocessor file all saved time steps will be automatically browsed through and listed. After a successful loading the postprocessor is positioned at the last saved time step. Any saved time step can be selected using **Browse file** button. The analyzing tools are similar to that of the simulator menu. The next graphics displays some of the visualization options which are available in the **View results** menu.

Notice: You can resize the diagram windows during the computation but the displayed diagrams will be refreshed and resized only when FEFLOW has free capacity. It is thus generally better to resize the windows before starting the numerical computation.

View results

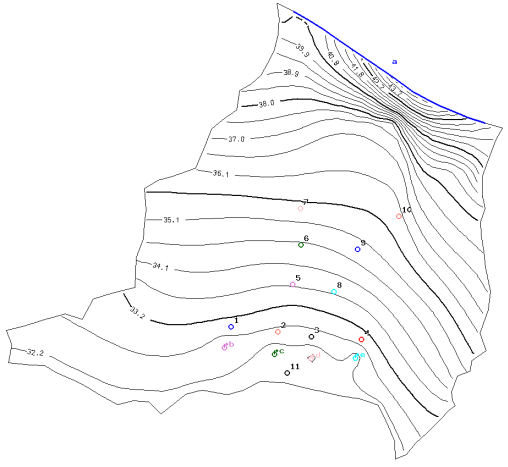
Use this option of the **Results viewer** for different time steps selected in the **Browse file** submenu.

Click on **Line sections & segments** to create some cross-sections for displaying the hydraulic head or mass distribution.

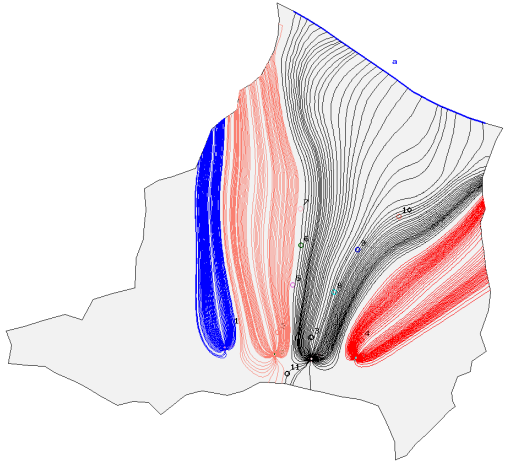
The backward particle tracking mode, using the multiple-pathline-around-single-well option, should give us an indication from which sites the contamination arrives at the wells.

Notice: Particle tracking is always performed based on the flow field at the current simulation time, treating the model as steady-state. All effects of time-varying pumping rates or time-varying recharge values are neglected.

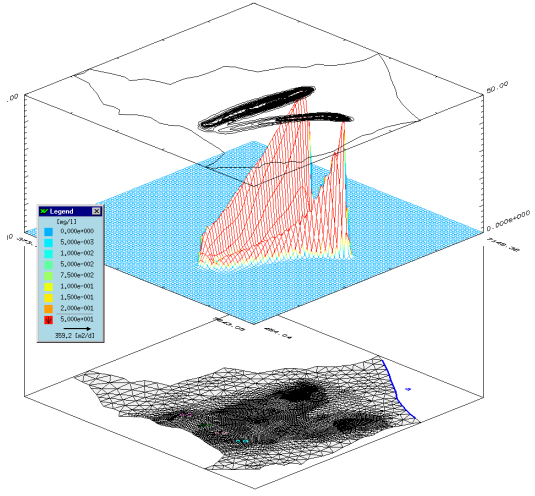
a)



b)



c)



d)

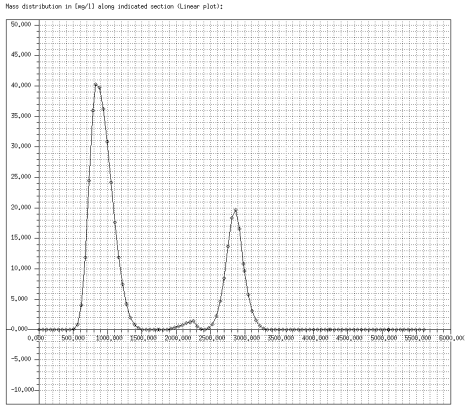


Figure 10.12 Visualization of the results: a) isolines, b) particle tracking, c) 3D projection, d) diagram.

Budget

The budget analyzer calculates in- and outflow for the inner and outer boundaries of the model including areal recharges (source/sink) for different time steps or over a time period. Try the various options, especially the balanced point groups and balancing for different time periods. Note that it is also possible to save the resulting budget values via **Save results in protocol file** to a commented ASCII file.

Have a closer look on the time development of the contaminant concentration in the different wells by using the grouped balance points. It is useful to estimate whether the contamination will increase after 1988 or not.

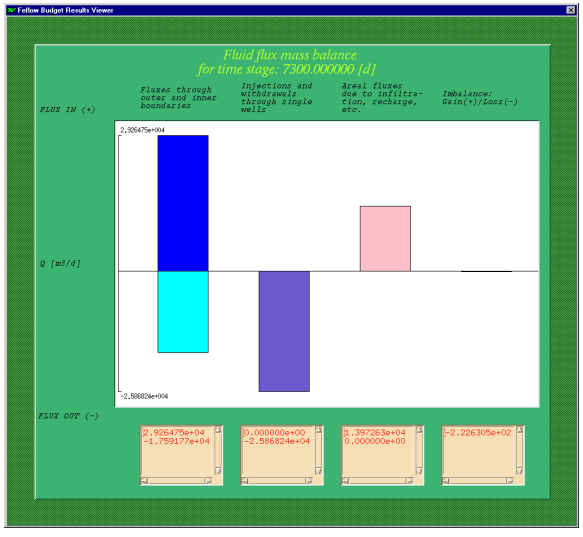

Fluid flux mass balance
for time stage: 7300.000000 [d]
Fluxes through outer and inner boundaries
Injections and withdrawals through single wells
Areal fluxes due to infiltration, recharge, etc.
Imbalance: Gain(+)/Loss(-)
FLUX IN (+)
Q [m3/d]
FLUX OUT (-)

Figure 10.13 Results of the budget analyzer.

Fluid flux analyzer

This tools gives information about Darcy velocities on single points and integrates in- and outflows for the whole model, subregions, lines, etc., even over time periods to be selected. As shown below the in- and outflows of water are displayed as cumulative curves.

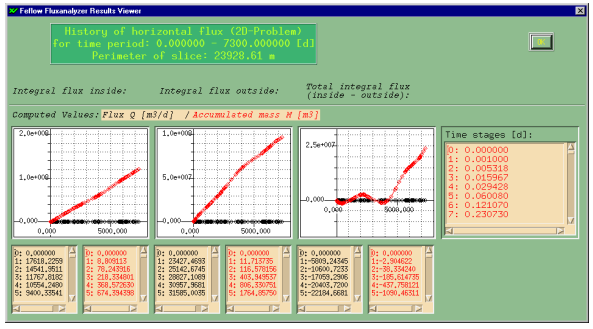

History of horizontal flux (2D-Problem)
for time period: 0.000000 - 7300.000000 [d]
Perimeter of slice: 23928.61 m
Integral flux inside:
Integral flux outside:
Total integral flux (inside - outside):
Computed Values: Flux Q [m3/d] / Accumulated mass M [m3]
Time stages [d]:

Figure 10.14 Results of the Fluid Flux Analyzer.

Calculate the outflowing amount of contaminant mass entering the lake and find the sections where the contaminant mass arrives at the lakeside by using the tools described above.

Temporal and spatial operations

This data operator menu allows useful manipulations of the resulting data in form of different temporal/spatial operations regarding differences, standard deviations or cumulative changes for time stages to be selected. The visualization of the results is done using the **Results viewer**.

Exporting data

Generally, data visualized in the **Results viewer** from the **Simulator** (Halt & View Results) and the **Postprocessor** (View Results)**,** but also in the **Flow**

***Notice**: The 'Fluid Flux Analyzer' calculates the fluid quantities on the base of the DARCY velocities at the nodes.*

data and **Transport data** menus via the **Special** tool, can be exported in two ways:

- **Data store manager** (DSM): You can choose different file formats and physical units for the data to be stored. Enter the DSM via the file selection box (Bu **Configure** button).
- **Capture**: The Capture function exports your drawing to a plot stack which can be read by FEPLOT, the plotting tool which comes with FEFLOW.

In the **Results viewer** menu select the Bu **Capture** button instead of the Bu **Show** button for saving a georeferenced FEFLOW plot (*.plx) file. You can add several plots to the same plot stack. Starting the **FEPLOT** tool via the **Print...** option of the **Quick access** menu (only on Windows NT/95) the last created plot file is visualized automatically and can be edited. UNIX users may install FEPLOT on a separate Windows PC and start FEPLOT from the WASY folder of the start menu. Alternatively, UNIX users may prefer to work with the **XPLOT** tool on UNIX, which you can start from the shell **Tools** menu. In XPLOT you can import all ASCII output files (points, lines, polygons), fpd files (file plot description files for color settings etc.) and HPGL background maps.

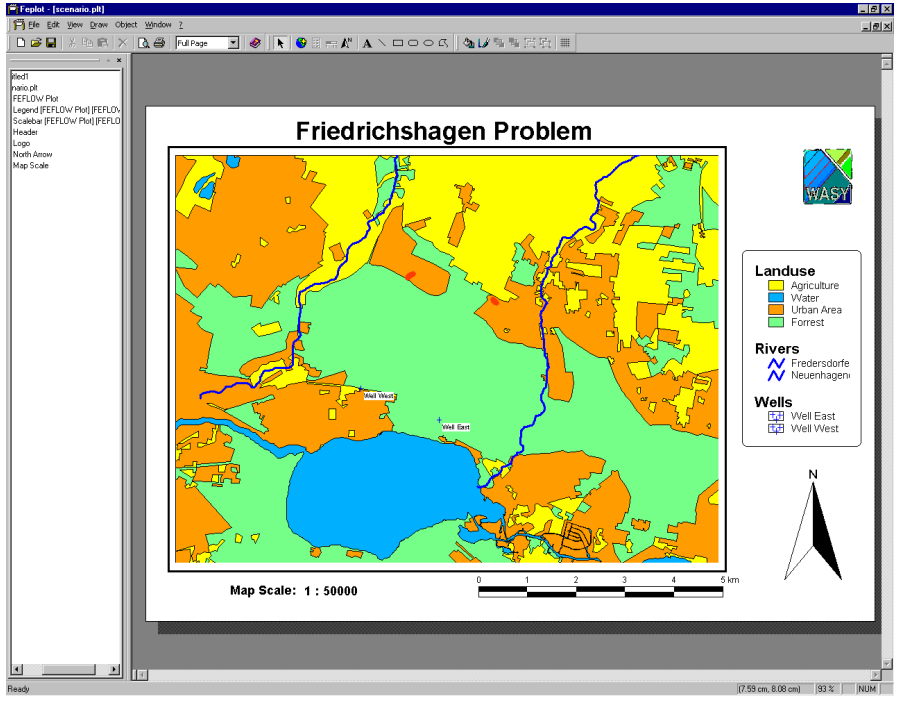


Figure 10.15 The plotting tool FEPLOT.

We have prepared a plot composition for FEPLOT which you can import:

- PC Users: Open the **Quick access** menu or the **File** shell menu and select the **Print..** option.
- UNIX Users: Start the PC where FEPLOT has been installed and click on the **FEPLOT** icon in the **Wasy** folder of the **Start menu**.
- **FEPLOT** starts and displays an empty page.
- Enter the **File** menu and select **Open..**. A file selector pops up.
- Choose the file scenario.plt from the **exercise\plot** directory. A so-called *map object* containing a view of the model area is displayed. A map object represents a georeferenced stack of files of different formats like ESRI shape file, ASCII topology files (Arc/Info and FEFLOW compatible) and FEFLOW *.plx plot files.

To overlay other files on the current map object

- Double click on the map object. The **Properties** menu pops up. You are in the *Layer* folder now. All currently loaded files are listed.
- Click on the **Add** button. A file selector menu pops up.
- Select the File type *ESRI shape* from the lower list, open the **import+export** directory.
- Select a shape file by double-clicking on its name
- A message box pops up asking to confirm. Click on **Okay**. The file is added to the map object.
- Click on **Okay** in order to leave the menu and to redraw the map object.

Figure 10.16 Drawing properties of a map object.

Once you have added a FEFLOW plot or a shape file you can control the visualization by classifying the attribute data:

- Click on the **Classify** button in the **Layer** folder of the **Properties** menu. The **Classifier** pops up.

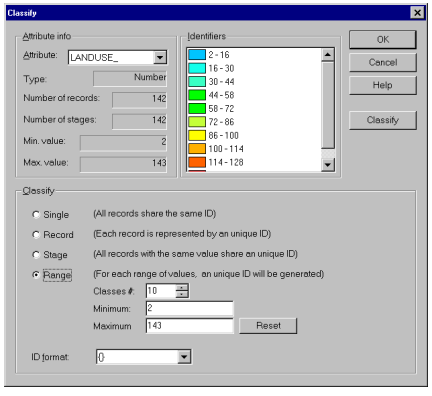


Figure 10.17 The classifier.

- In the upper left *Attribute info* field select the *Attribute* you want to classify. Below, information of the attribute type and the data is given.
- In the lower *Classify field* you can specify how you want to classify the data. Hit <F1> for detailed information.
- At last click on the **Classify** button. The classification is shown in the *Identifiers* list.
- Leave the menu clicking on the **Okay** buttons.

To create a new map object

- Click on the **Globe icon** in the **Tool bar**.
- Click within the working window to set the first corner of the map object.
- Hold the left mouse button pressed and open a rectangle by dragging the cursor across the working window.
- Release the left mouse button. The **Properties** menu pops up.
- Click on **Add** for adding files to the map object as described above.
- Leave the menu clicking on the **Okay** buttons. The new map object is shown on the working window.

Other items in the **Properties** menu control the scale, the colors and outlines of the visualized data, the background settings and the exact position of the map object on the page. Invoke the FEPLOT online **Help** by hitting <F1> for detailed information. You can print the plot using the standard Windows print interface. Leave FEPLOT and return to FEFLOW.

As an alternative to FEPLOT you can use the GIS System ArcView from ESRI or the CAD system AutoCAD for plotting your results and for further analysis of the resulting data. Model data can be exported in shape-file format (*.shp) or AutoCAD file format (*.dxf) using the Data Store Manager (DSM).

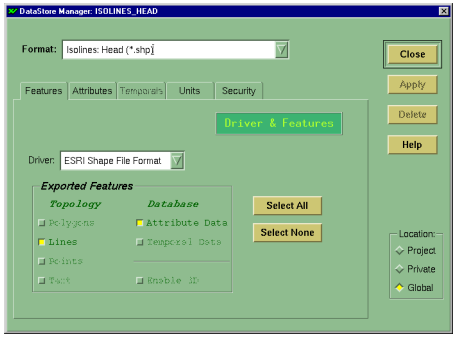


Figure 10.18 The Data Store Manager (DSM).

For example, click **Isolines** - **Fringes** in the dark red square of the **View results** window. Choose the **Configure** button in the file-selection dialog to enter the DSM. Using the different tabs you can:

- select the file format,
- control the exported database items,
- change units and,
- define file permissions.

Return to the file selector pushing the **Close** button and store the file.

10.3.6 Conclusions for the 2D model

As the simulation reveals, both sites are potential contaminators of the wells. Obviously, the sewage plant is a stronger potential contaminator and seems to affect the two center wells. In contrast, the waste-deposit site seems to only influence the contaminant concentration of the mid-east well. Considering the fact that the contaminant plumes merge before arriving at the wells, it cannot be stated exactly which contaminator affects which well.

To distinguish more clearly between the two sites it seems necessary to describe more realistically the complex hydrogeologic situation of the area. Specifically, we should attempt to solve the problem by creating a three-dimensional model of the study area as described in the next chapter.

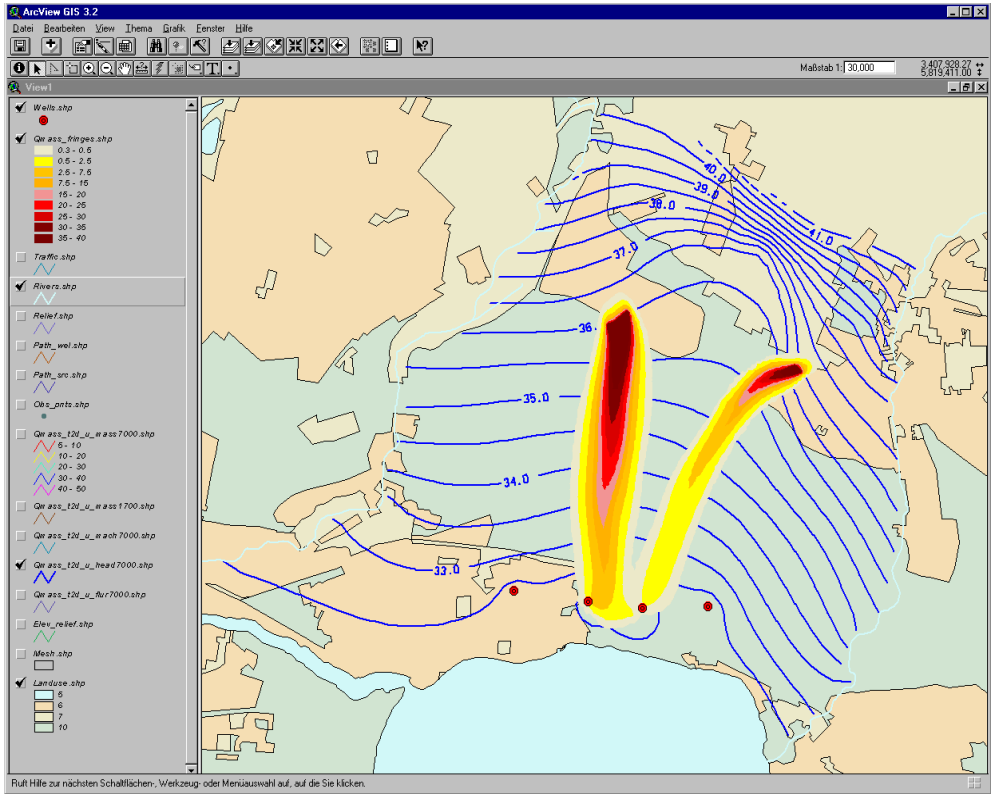


Figure 10.19 Visualization of the contaminant plumes in ArcView.

10.4 The 3D Model

In analyzing the results of the 2D model we found that both examined sites could be responsible for the groundwater pollution. To obtain more detailed results we now want to account for the complex geologic situation by extending our model to the third dimension. For this tutorial we will create an unconfined, steady flow and steady transport problem.

10.4.1 How to get the data

The input of stratigraphic information can be done via the same tools which you have used in the flow data menus. For transferring the stratigraphy to the 3D model in FEFLOW a conceptual model should be available. Often you get the basic information from borehole data. These data are used for creating vertical profiles and, finally, for the complete 3D conceptual model of the study area.

10.4.2 Step 1 - Designing slices and layers

Enter the **Layer configurator** via the **Dimensions** shell menu selecting the *Three-dimensional (3D)* command.

The configuration of the layers and slices as well as the geometric relations are defined in the **Layer configurator**. You can enter the **Layer configurator** via the **3D-slice elevations** menu of the **Problem editor**, too. The geometry of a 3D model is built up by slices and layers (Figure 10.20).

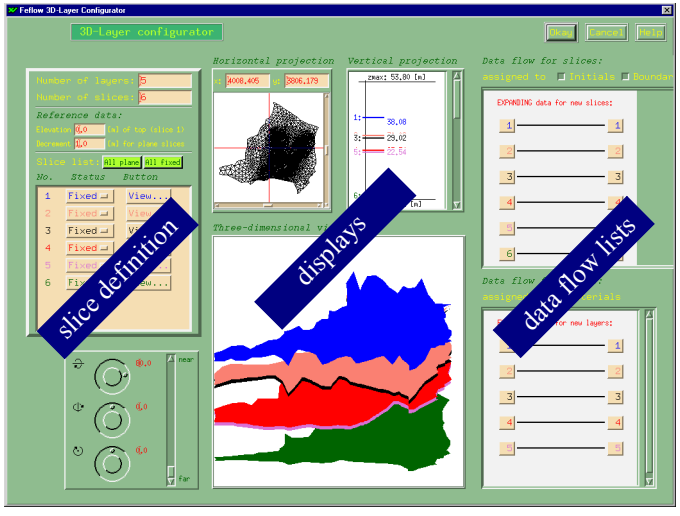


Figure 10.20 3D-Layer configurator.

Slices

Slices are surfaces on which the finite element nodes are located. They represent the topography and the discontinuities between the stratigraphic units or just subdivide layers to refine the vertical spatial discretization.

On **slices** you assign

- **Initial conditions** and,
- **Boundary conditions**.

Layers

Each layer is bounded by two slices. Layers contain the **Material properties**. *For the construction of 3 layers you need 4 slices*. Model layers represent the stratigraphic layers and their subdivisions. In particular cases a layer also can be considered as initially dry (so-called 'air-layer') which is useful to model free-surface problems such as mine flooding.

On **layers** you assign

- **Material parameters**.

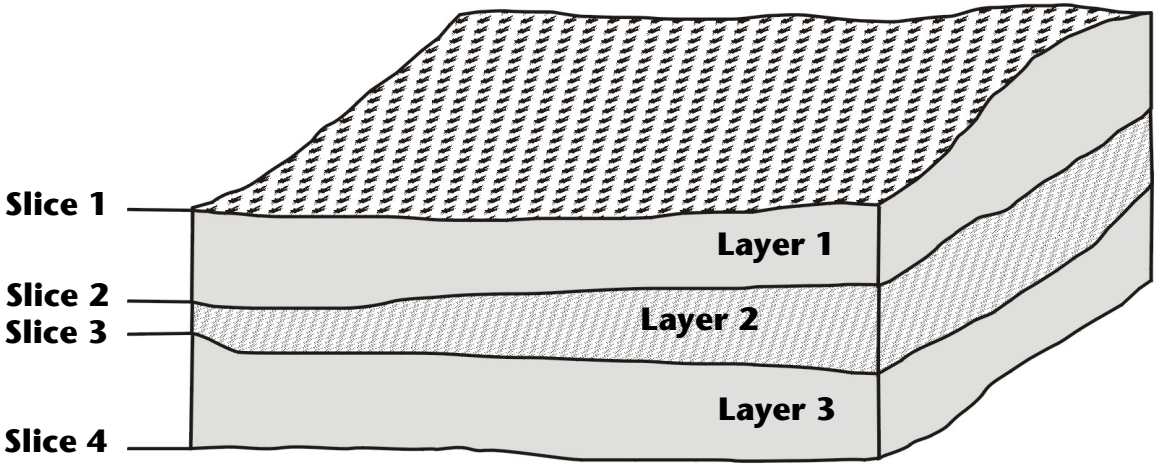


Figure 10.21 Schematic view of a model - slices and layers.

Now you have to define how many layers/slices you need: The upper aquifer is limited by the ground surface at the top and by an aquitard at the bottom. The second aquifer is situated below that aquitard, underlain by a till layer of unknown vertical extension. First we create the slices necessary for the description of the stratigraphy.

Set all slices in the *Slice list* on **Plane**, which allows to edit their vertical position freely.

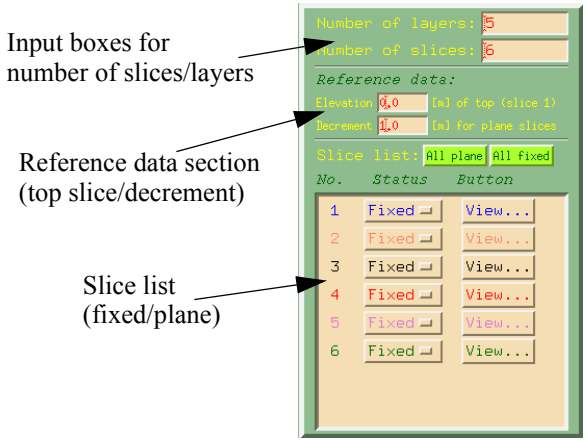

Input boxes for number of slices/layers
Reference data section (top slice/decrement)
Slice list (fixed/plane)
Number of layers: 5
Number of slices: 6
Reference data:
Elevation 0.0 [m] of top (slice 1)
Decrement 1.0 [m] for plane slices
Slice list: All plane All fixed
No. Status Button
1 Fixed View...
2 Fixed View...
3 Fixed View...
4 Fixed View...
5 Fixed View...
6 Fixed View...

Figure 10.22 Slice definition (cut-out).

Enter an *Elevation of top slice* of **10000** m and a *Decrement* of **100** m in the *Reference data section* (Figure 10.22). This should be sufficient to precisely re-assign the stratigraphic data for each slice later without running the risk of interfering with previous slices. Create three layers (four slices) by entering the value in the corresponding 100 input field (Figure 10.22) and hitting <Enter>. The **Slice partitioner** pops up (Figure 10.23) where you can decide where the new slices should be positioned (Figure 10.23 a, c); place them below the bottom slice.

Next we should have a look at the data-flow diagrams to the right of the layer configurator. It shows that the slice information of the former top slice/layer is inherited by the new one. The same is valid for the bottom slice/layer.

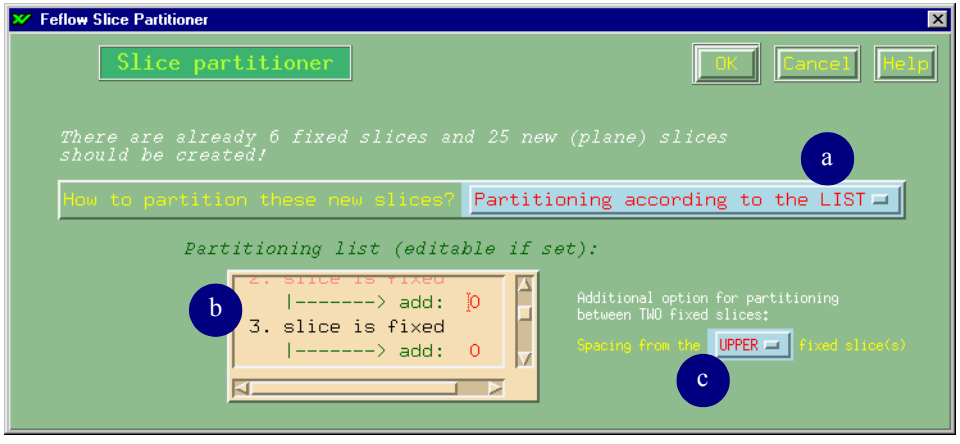


Figure 10.23 Slice partitioner a) how to partition the new slices, b) partitioning list, c) select reference slice for spacing.

10.4.2.1 3D Slice elevation

Leave the **Layer configurator** via the **Okay** button. The explicit assigning of z-elevations for every node at a slice is done via the **3D-slice elevation menu** of the **Problem editor**. Here you can select every slice and assign the z-elevations using the standard tools of FEFLOW.

Select the slices by clicking on the corresponding numbers in the *layers & slices browser* and Assign (Akima linear, 0% over- undershooting) the databases according to the list (Table 10.7). Start with the lowest slice in order to avoid intersections with the other slices. In case of an intersection due to the interpolation method an alert box pops up offering to insert a minimum decrement between the intersecting slices at the critical nodes.

Table 10.7 z-elevations database

slice	database
4 (bottom slice)	bot_san2.trp
3	bot_clay.trp
2	bot_san1.trp
1 (top slice)	relief.trp

10.4.2.2 Reconfigure 3D task

The basic stratigraphy is now complete. We want to insert two additional slices because of the large contrast in conductivity between the aquitard and the aquifers. Specifically, we will create two thin **buffers** at the top and the bottom of the aquitard.

Re-enter the layer configurator by clicking on **Reconfigure 3D task**. We recommend to design the problem as follows:

Set all slices to *fixed* in the slice list, i.e., the z-elevations of these slices won't be changed during the reconfiguration of the aquifer layering.

Type a decrement of 1 m in the **Reference data** *decrement* box (Figure 10.22).

First we insert a slice for creating the upper buffer. The slice should have the set decrement measured from the top of the aquitard (the buffers will belong to the aquitard stratigraphically).

Change the number of slices from 4 to 5 in the slice box (Figure 10.22) and hit <Enter>.

In the pop-up **Slice partitioner** menu choose the *Insert slices according to the list* mode (Figure 10.23 a) and make sure that the small button at the right is set to „decrement measured from the *upper* slice" (Figure 10.23 b).

Delete the "1" automatically set by FEFLOW under the bottom slice and replace the "0" by a "1" to insert the new slice between the 2nd and 3rd existing slices.

Click Okay.

Set the new slice to *fixed* in the slice list.

Repeat the procedure for a sixth slice to be inserted between the 3rd and 4th slice, using a decrement measured from the *lower* slice (bottom of aquitard).

The data flow to the new slices can be checked and modified by the two menus to the right of the layer configurator, the data flow lists. The upper list defines how boundary and initial conditions should be inherited, the lower menu controls the material parameters. The numbers in the left column symbolize the old slices or layers, the right column contains the new ones. For inheriting data

- Click on the old slice or layer as data source.
- Click on the new slice or layer as data target.

***Notice**: For every node on a slice only one z-elevation can be assigned.*

A connecting line is drawn symbolizing the data transfer. You can transfer data from one slice or layer to several slices or layers.

Make sure that the new slices get the data of the aquitard.

10.4.3 Step 2 - Assignment and control in the problem editor

After having defined the basic stratigraphy and having added the buffers we need to reassign some problem attributes and control the data flow. Return to the **Problem editor** menu.

10.4.3.1 Problem class

The **Problem class** remains on *Transient flow/transient transport* of an *Unconfined* aquifer for fully *Saturated* media.

Click on the **Edit free surface(s)** button in the lower part of the menu. The **Free surface(s) editor** pops up. Here you can define the hydraulic properties of the slices.

We will use the **BASD** technique for this simulation. For the theory of the **Best-adaptation-to-stratigraphic-data** method see the Reference Manual (Section 2.4). Using the BASD technique the finite element mesh is adapted in the z-direction in according to the movement of the upper water table as described by the hydraulic head at the top slice. All inner slices also change their vertical positions; FEFLOW computes their respective optimum position so as to maintain the stratigraphy-related information without smoothing (interpolating) the data from adjacent layers. In other words, it finds the best adaptation to the stratigraphic data. Only slices set to *fixed* or *phreatic* will not be moved. This technique is often useful in modeling multi-layer aquifer systems. The following slice types can be set:

- **Free & movable**: Only the top slice for free surface problems, BASD automatically activated.
- **Phreatic**: Defines the top of an unconfined aquifer; the slice cannot move and should be separated from a free & movable slice by a fixed slice.
- **Fixed**: Slice defines the top of a confined aquifer or an aquitard. It cannot move. A free & movable slice cannot move below a fixed slice in case of an overlaying aquifer falling dry, instead natural constraints are activated that force the water table to remain above the fixed slice (Reference Manual, Part I).
- **Unspecified**: For movable meshes FEFLOW adapts the slice automatically depending on the definition of the adjacent slices. This setting is meaningless for fixed slices.

Set the slices so that the upper layer is unconfined and movable while the lower aquifer is confined (free & movable, unspecified, unspecified, fixed, unspecified, fixed).

Now leave the **Problem class** menu.

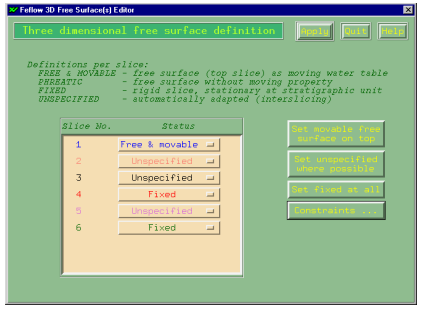


Figure 10.24 Three-dimensional free surface definition.

10.4.3.2 Flow initials

Make sure that the flow initials are set on every slice. Use the **Copy** tool (below the Assign tool, light blue button) if initials are missing on slices.

10.4.3.3 Flow boundaries

- 1st kind: applied only to the upper two slices. Use the **Erase** button for the remaining slices;
- 2nd kind: on every slice belonging to an aquifer, not on slice 3 and 4;
- 3rd kind: on the two upper slices.
- 4th kind: We will create some **multi-layer wells**, i.e., wells which extract water from both aquifers.

FEFLOW can connect the well boundary conditions on adjacent slices. To activate this function you have to set the corresponding button in the **Special options settings...** submenu of the shell's **Options** menu. Set the wells as shown in Table 10.8. Well *West* only extracts water from the first two slices. The recharge rate has to be assigned to one node and is automatically distributed to all connected (adjacent) well boundary conditions according to the multi-layer characteristics. Well *MidWest* has defined pumping rates for every slice in both aquifers, instead. Well *Mid East* is screened over the full length, Well *East* only in the lower aquifer.

Table 10.8 Pumping rates for multi-layer wells

slice No	Well West [m^3/d]	Well MidWest [m^3/d]	Well MidEast [m^3/d]	Well East [m^3/d]
1	4200	1550	6200	-
2	0	1550	0	-
3	-	-	0	-
4	-	-	0	-
5	-	1550	0	4200
6	-	1550	0	-

Flow Materials

Assign values for the conductivities of the layers according to the values in Table 10.9 for *Kxx*, *Kyy*, and *Kzz*.

For defining the hydrogeologic window connecting the two aquifers as described in the **Scenario** description (Section 10.2) select layer 2 and import the polygon clayhole.ply via the **Join** tool (Const.). For the area defined by that polygon, set *Kxx* to **1.0e-03** m/s (remember that the default unit is 1e-4 m/s!). Select the **Copy** tool and copy the values of *Kxx* to *Kyy*, *Kzz*, respectively (*Advanced* option in the **Copy** menu) and to the layers 3 and 4 which form a part of the aquitard, too (*Layer-related* option in the **Copy** menu). The storage compressibility should be set to a small value for the aquitard.

Table 10.9 Additional flow material settings for 3D

Layer No	*Kxx*	*Kyy*	*Kzz*
Layer 1	conduc2d.trp	conduc2d.trp	conduc2d.trp
Layer 2	1.0e-06 [m/s]	1.0e-06 [m/s]	1.0e-07 [m/s]
Layer 3	1.0e-06 [m/s]	1.0e-06 [m/s]	1.0e-07 [m/s]
Layer 4	1.0e-06 [m/s]	1.0e-06 [m/s]	1.0e-07 [m/s]
Layer 5	1.0e-03 [m/s]	1.0e-03 [m/s]	1.0e-03 [m/s]

10.4.3.4 Assigning and checking the transport data

Mass Transport Initials

No changes are necessary.

Mass Transport Boundaries

The contaminant mass conditions are applied only at the top slice. Bu Erase the contaminant sites from the second slice and Copy those parameter settings to the underlaying slices. The “freshwater” boundary conditions should only remain at the border sections where flow boundary conditions are imposed!

Mass Materials

Change the **Porosity** for the clay (aquitard) to **0.05**, except for the area with the hydrogeologic window (**0.2**). The storativity of the lower aquifer should be set to **0.2**, too.

You can now run the simulation. Do not forget to save the FEM file before running, otherwise the initial distributions for hydraulic head and mass concentration will be lost once the simulation starts. Save the simulation output in a DAC file via the options of the **Control output** menu of the simulator. Be sure to define all desired Bu **Control output** settings before starting the simulation run.

10.4.4 Step 3 - Postprocessing in 3D

After the simulation has finished, enter the **Postprocessor**. You can load the prepared 3D dac file q_mass_3d_tu.dac or the file just created during the simulation. The menu items of the Postprocessor are the same as for 2D models (with some items providing additional options in 3D).

Start with the **Results viewer** (View results).

10.4.4.1 Results viewer

In 3D always the currently active slice is analyzed. You can browse the slices using the **Layers & slices** browser (Figure 10.26) at the lower left side of the **Working window**.

There are some additional options for cross-sectional analysis compared to the possibilities in 2D.

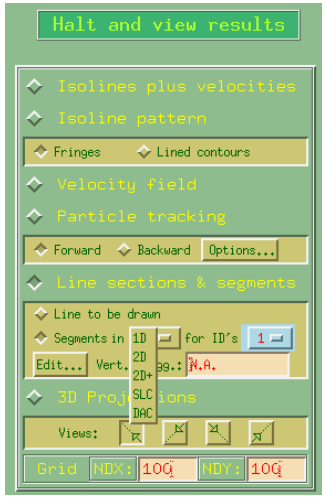


Figure 10.25 Results viewer.

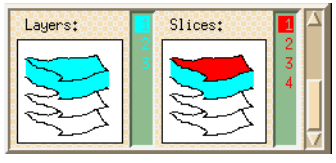


Figure 10.26 Layers & slices browser.

Line sections & segments

Create new segments for cross sections via the **Edit** - *Draw Segments* option. Check the 2D, 2D+ and SLC options of the **Segments** tool by switching the light blue toggle. Choose between lined contours or fringed isolines by selecting the corresponding items of the Isoline pattern option above. The DAC option for line sections allows to save a cross-section as a complete results file for reducing the problem to a 2D vertical model.

10.4.4.2 Budget menu

The **Budget** menu offers additional options to analyze the current slice, a list of slices, or the whole model domain. Here, we check the different in- and outfluxes for the two aquifers. Do the results correspond with the ones previously obtained by the 2D model? How are the mass-flux quantities in the two aquifers related to the different contaminators (use the slice list for selecting the two aquifers separately)?

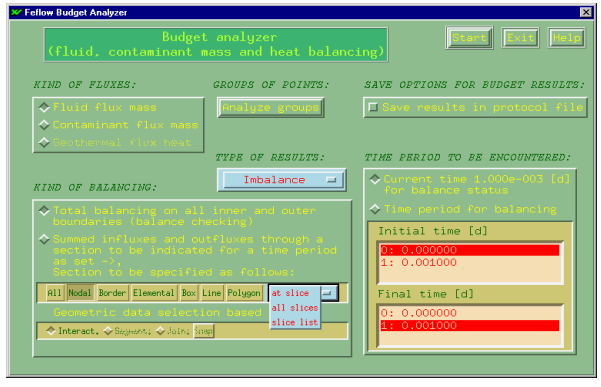


Figure 10.27 Budget analyzer.

10.4.4.3 Fluid-flux analyzer

Using the flux analyzer we can quantify the flows through the model or through a subarea in vertical or horizontal direction. The fluxes are computed from the Darcy velocity and the corresponding area, either node-wise (continuous) or elementwise (discontinuous).

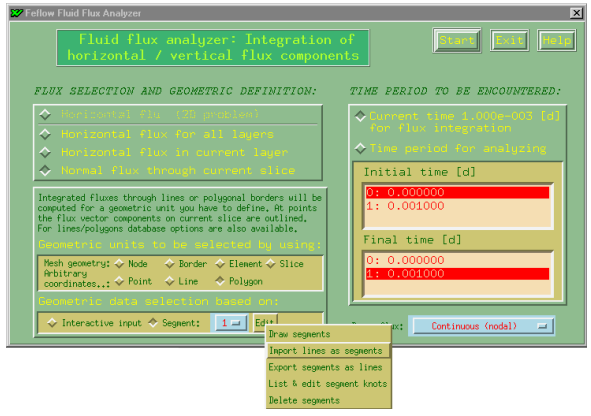

Feflow Fluid Flux Analyzer
Fluid flux analyzer: Integration of horizontal / vertical flux components
Start
Exit
Help
FLUX SELECTION AND GEOMETRIC DEFINITION:
TIME PERIOD TO BE ENCOUNTERED:
Horizontal flux (2D problem)
Horizontal flux for all layers
Horizontal flux in current layer
Normal flux through current slice
Current time 1.000e-003 [d] for flux integration
Time period for analyzing
Initial time [d]
0: 0.000000
1: 0.001000
Final time [d]
0: 0.000000
1: 0.001000
Integrated fluxes through lines or polygonal borders will be computed for a geometric unit you have to define. At points the flux vector components on current slice are outlined. For lines/polygons database options are also available.
Geometric units to be selected by using:
Mesh geometry: Node Border Element Slice
Arbitrary coordinates..: Point Line Polygon
Geometric data selection based on:
Interactive input
Segment:
Edit
Continuous (nodal)
Draw segments
Import lines as segments
Export segments as lines
List & edit segment knots
Delete segments

Figure 10.28 Fluid flux analyzer.

We want to check how much water is flowing through the hydrogeologic window.

Use the corresponding background map for this subarea (clayhole.ply) as template.

Polygons cannot be imported explicitly into this menu, so we insert the polygon as **Segment** and use it for the flux analysis:

- Select **Normal flux through current slice**.
- Geometric units to be selected: **Polygon**.
- Geometric data selection based on: **Segment**. The **Edit** button becomes enabled.
- Click on **Edit** and
- Select **Import segments as lines.** The **File Selector** pops up. In the uppermost field, the **Filter**, the extension ***.lin** is shown**.**
- Change the extension to ***.ply** and
- Click on the **Filter** button at the lower edge of the file selector.
- Select the file clayhole.ply and click on **Okay**. The polygon is imported and visualized as colored line with an ID.
- Select the **ID** from the light blue button and
- Click **Start**.

10.4.5 Step 4 - 3D Options menu

For visualizing 3D problems FEFLOW provides the **3D Options** menu. You can enter that menu from the *Shell* menu as well as from the *Problem Editor* for visualizing the parameters already set or from the *Simulator* menu and from the *Postprocessor* where additional analyzing tools are available. Use the **Tricycler** for manipulating the display and move the visualized objects by mouse.

Perform the simulation run with the extended model and enter the **3DOptions** menu (green button on lower left side of the screen, Figure 10.30).

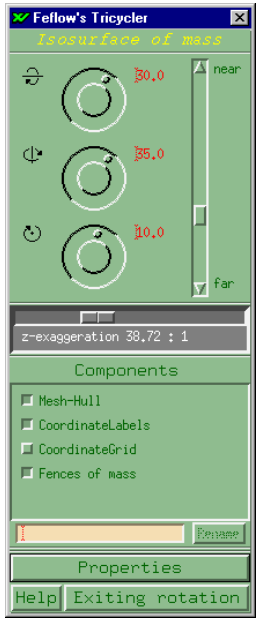


Figure 10.29 Tricycler.

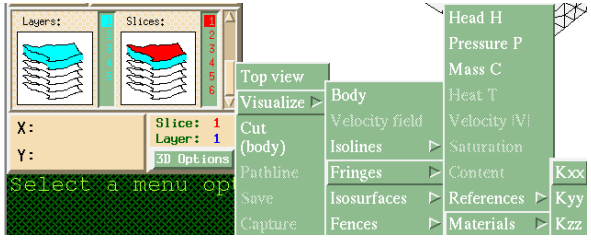


Figure 10.30 3D Options menu.

Visualize

Select Visualize - Fences - Materials - *Kxx* (see Figure 10.30) to get a view of the distribution of conductivity values along the previously designed fences and segments.

Change the value of *Isosurface scalar,* to, for example, **10,** in the **Tricycler** (**Properties** - *General*)**.** Afterwards enter the **3D Options** menu and select Visualize - Isosurface - Mass C. The 10 mg/l isosurface for contaminant mass will be visualized.

Try the visualization of the other options, too. What would you get by visualizing the 0 kPa isosurface of pressure?

Try to switch parts of the visualization on and off using the checkboxes in the **Components** list and test the changing of colors (**Properties** - *Color*).

Cut (body)

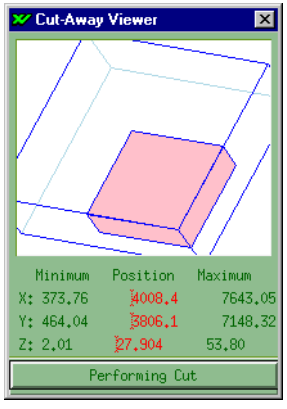


Figure 10.31 Cut-away viewer.

Press **Exit rotation** and start the 3D visualization again, for example with **Fringes** for **Mass C**. Click again on the **3D Options** button and select **Cut (body)**. You can define a cut-out either by typing the coordinates in the corresponding fields of the *Cut-away Viewer* (see Figure 10.31) or by moving the red handlers in the 3D view. Try to find the area where the hydrogeologic window is located and click on the

Performing cut button.

Pathlines (RAI)

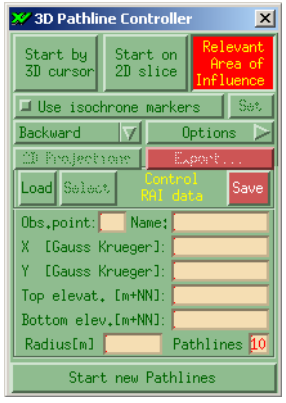


Figure 10.32 3D pathline controller.

Close the visualization again and choose the **Pathlines** option from the 3D-Options menu. Select **Relevant area of influence** (RAI) in the popped up *Pathline-Controller*. This option starts the computation of pathlines, in backward direction starting from a circle with defined diameter around the upper and lower edge of the screen of a well. Select **Load** in the *Control RAI data* section to import the necessary information from a special database named wells.rai.

A submenu pops up displaying the database. Select one well and start the pathline computation. You can export the results as **2D projections** in different file formats (using the Data Store Manager) or as 3D screen dump (hit <Alt>+<X> on UNIX, <Alt>+ <Print> on PC). Manipulate the setting of the **isochrone markers** (**Set**) and change the default **Options** for the Pathline Outfit.

After having analyzed the model and stored the results exit the 3D Options menu by clicking on **Exiting rotation** in the Tricycler window.

10.4.6 Final remarks

The simulation of the 3D model shows a much more complex situation than the 2D model had indicated. The aquitard leads to different migration paths of the contaminant plumes in the two aquifers. For the model to better reflect the reality, it would seem prudent to take one more step: the temporal variance of the data should be incorporated. The assigning procedure is basically the same as for the transient 2D model. If you have questions, please refer to the context-sensitive online **Help** which is invoked by hitting <F1> or clicking on the 'Help' button. To better understand the theoretical background of the modeling approach and its implementation in FEFLOW, please consult the Reference Manual. If you have any further questions please contact your local distributor

10.5 List of files

Table 10.10 List of all files for importing problem-specific data in FEFLOW

Parameter	File name	Description
Mesh Editor		
Background maps	rivers.lin, landuse.lin, geology.lin, model_area.lin,	Line files as active templates for the designing of the superelement mesh, mesh refining etc.
Mesh Generator		
Mesh Geometry	refine_region.ply	Polygon file for areal mesh refining by A-Join
Temporal & Control Data		
Time varying pumping rates	well_rates.pow	Time-function value curve for the pumping rates of the four wells
Flow Data		
Flow initials	head_ini.trp	Initials of hydraulic head
Flow Boundaries		
1st kind	wlevel_s.trp	Hydraulic head for lake surface
3rd kind	wlevel_w.trp wlevel_e.trp	Reference hydraulic heads for rivers
4th kind	mean_well_rate.trp well_time_funcs.trp	Location and pumping rates/power-function IDs of the wells
Flow Materials		
Conductivity (Transmissivity)	conduc_2d.trp (trans_2d.trp)	x-y-fvalue file for data regionalization of conductivity
z-elevation files	relief.trp bot_san1.trp bot_clay.trp bot_san2.trp	x-y-fvalue file for data regionalization of the aquifer geometry (2D) and slice elevations

Table 10.10 List of all files for importing problem-specific data in FEFLOW (continued)

Parameter	File name	Description
Source(+)/Sink(-)	mean_recharge.ply mean_recharge.dat time_recharge.ply time_recharge.dat	Polygons (*.ply) and ASCII databases (*.dat) for joining of groundwater recharge
Transport Data		
Transport Boundaries		
1st kind	mass_source.lin	File defining the position of the contaminant sources
Reference Data		
Observation points	obs_pnts.pnt	Observation points
Fences/Sections	fences.lin	Lines for creating cross sections etc.

Table 10.11 Default directory names

Directory	Contents	file formats
supermsh	Superelement mesh data	*.smh
femdata	Finite element problem data	*.fem
results	Resulting data	*.dac, *.dar
plot	Plot files	*.fpd, *.fpc, *.plx, *.plt
import+export	Import & export files	*.pnt, *.lin, *.ply, *.shp, *.tif, *.pow, *.trp, *.dat

Part III

Interface Manager

Programming Interface

11

11.1 Introduction

The majority of FEFLOW users may prefer its compactness, to have all tools for preprocessing, simulation, postprocessing, and data analysis combined under the same graphical surface.

But under some circumstances it can be necessary to have more user control over simulation, data regionalization, visualization, and more. For these cases FEFLOW provides a tool called Interface Manager (IFM). The IFM manages an arbitrary number of external modules. Any installed, registered, and activated module can access FEFLOW's internal data storage and method pool via a published programming interface (API). To classify the different situations (contexts) of calling modules, FEFLOW provides a special interface for each context. Basic interfaces are Simulation and Regionalization. Depending on the principle of integration with FEFLOW's internal methods, two basic types of interfaces can be distinguished: (1) the external module replaces FEFLOW-internal methods (Figure 11.1) or (2) the external module extends the internal functionality (Figure 11.2).

With the software technology of Shared Libraries, or Dynamic shared objects (DSO) under UNIX or Dynamic Link Libraries (DLL) under Microsoft Windows, it is possible to extend FEFLOW's functionality without modifying its source code, which would cause licensing issues. Neither object code nor any libraries are necessary since the IFM uses a jump-table technique which can be provided in source code. The implementation of these jump tables lies completely on the side of FEFLOW. Therefore, modules have no external references to FEFLOW's code or data. Changes inside FEFLOW will not affect the functionality provided by the module. Thus, a module does not depend on a particular FEFLOW version but is responsible for its own version management. A group of API functions provided by the IFM supports the creation and management of downward and upward compatible modules.

The extension of FEFLOW by modules can be of interest for users who have no intention to write own source code but want to use extended functionality provided by already compiled and linked modules. Another group, the programmers, has developed some own specific software and want to use it in FEFLOW's environment.

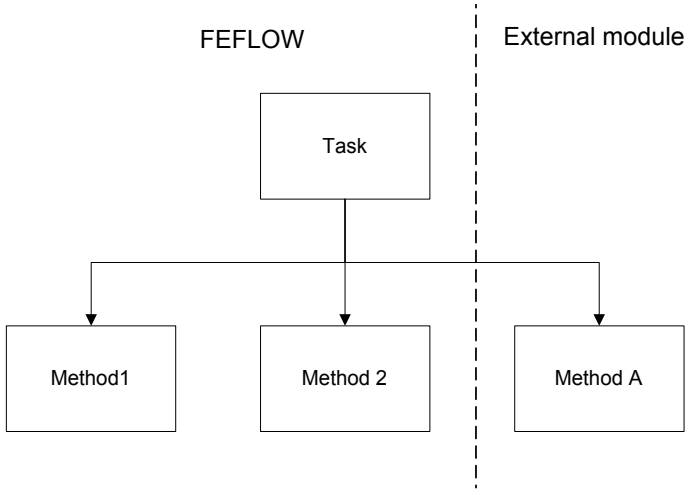


Figure 11.1 Replacing internal methods (e.g., *regionalization*).

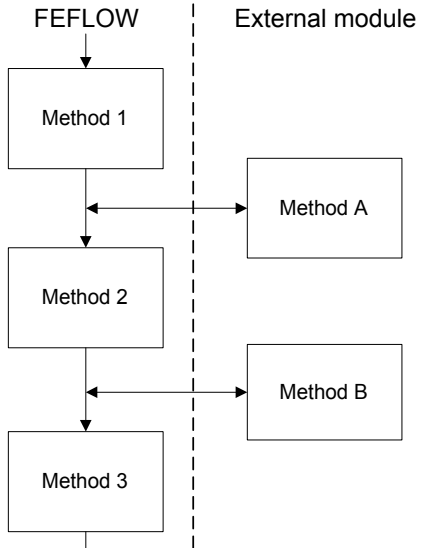


Figure 11.2 Extending internal methods (e.g., *simulation*)**.**

For the first group it becomes very easy: simply registering the module at its location. According to the interface specification inside the module it will be integrated in FEFLOW's graphical environment. Through additional interface elements like buttons, lists, etc. the user can select among both built-in and module-provided functionality.

For programmers FEFLOW provides the Interface Manager as a comfortable CASE tool for:

- Creating and managing projects to build FEFLOW-conform modules,
- Generating source code for module registration and for all module entry points (callbacks),
- Saving and loading module-related data into and from FEM files,
- Calling selectively the module for interface-specific events,
- Getting and setting FEM problem data (materials, boundary conditions, results),
- Using FEFLOW's graphical environment for data displaying,
- Using FEFLOW's HTML based help system for documentation,
- Popping up own dialogs for graphical user interaction,
- Saving and restoring-module-related user preferences in a personal profile.

An interface consists of a set of available callback functions. Each callback function, or callback for short, will be called from a different point of FEFLOW's program flow. For instance, the callback PreTimeStep will be called immediately before the simulation loop starts a new time step. Refer to the FEFLOW online help for a complete reference to all supported callback functions available in each interface.

An arbitrary number of modules can be registered for each interface. A module does not have to implement all callbacks provided by the associated interface, but only those of actually used by the module. In the process of module development it is common to start with few implemented callbacks and to increase the number according to the growing functionality requirements.

The next section describes how to use the Interface Manager for adding existing modules.

11.1.1 Common terms

Table 11.1 Common terms

Term	Explanation
Interface Manager	(1) Set of API functions and callback definitions necessary for writing own modules; (2) Module administration dialog inside FEFLOW.
Module	A shared library or Dynamic Shared Object (DSO) under UNIX or a Dynamic Link Library (DLL) under Microsoft Windows containing automatically generated code (module stubs code) and user-written code.
Interface	Defines the context of calling external functions. Current interfaces are *Simulation* and *Data regionalization*.
Callback	As FEFLOW uses modules in an event-driven manner each entry point of a module represents a callback function. Typical callbacks are *OnBeginDocument*, *Serialize*, or *PreTimeStep*.

11.1.2 Abbreviations

Table 11.2 Abbreviations

Abbreviation	Meaning
$FEFLOW_HOME	Installation directory of the FEFLOW package
2D	Two-dimensional
3D	Three-dimensional
API	Application Programming Interface
CASE	Computer-Aided Software Engineering
DLL	Dynamic Link Library
DSO	Dynamic Shared Object (shared library)
FEM	Finite-Element Method
GUI	Graphical User Interface

Table 11.2 Abbreviations (continued)

HTML	Hypertext Markup Language
IFM	Interface Manager
MS Windows	Microsoft Windows NT/ 2000/XP or 98/ME
X11	Body Window System of UNIX

11.2 Interface Manager for Users

11.2.1 Module configuration

The administration of modules is part of the IFM dialog called from the main-menu entry 'IFM' - 'Configure'.

With the selection of an interface in the left column all registered modules for this interface are displayed in the middle column while the right column shows all events (callbacks) for which a module can be called. After selecting a module all implemented functions are marked in the right column with a plus sign (+) and all non-implemented functions with a minus sign (-). The top section shows the prototype and a short explanation of the callback function.

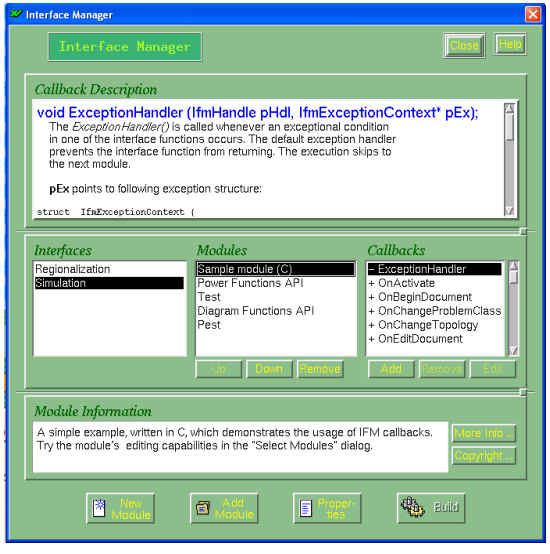


Figure 11.3 Configuration dialog.

For the selected module you will find a short overview in the Module-information part of the dialog. By pressing the "More info..". button you can raise a detailed description. With the 'Copyright' button the copyright note of the module becomes visible.

From the button bar you reach the dialogs for creating a 'New Module' (project), adding an existing module ('Add Module'), and modifying the module Properties (name, files, parameters, etc.) The 'Build' button starts the compilation and link process (UNIX/Linux only). As the result, the shared library of the module will be generated.

11.2.2 Registering a module

Note that for registering a module only available in source code we refer to the complete IFM manual on your FEFLOW CD.

Before a module can be used it must be registered in FEFLOW. To register an existing module open a file selection dialog with the Add Module button (see Figure beside) and browse for the desired module. Once the path of the module is selected and the dialog has been closed by pushing the OK button, the IFM attempts to load the module DSO (DLL). If

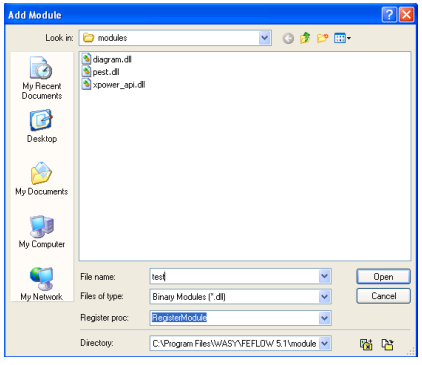


Figure 11.4 File selection box.

***Notice**: Programmers are kindly asked to print the full Programming Interface manual from the CD and to use the detailed context sensitive online Help.*

successful, the IFM tries to resolve the symbol specified in the 'Register proc' field. By default, all modules should provide the routine 'RegisterModule'. Otherwise you have to obtain the name of the registration function through additional information, like a README file, a letter, etc.

11.2.3 Module properties

Usually, the module properties dialog of a binary format module is read-only because changing of properties would require the recompilation of the module (Figure 11.5). However, you can use the dialog to enter a new module location after the module has been moved to another directory.

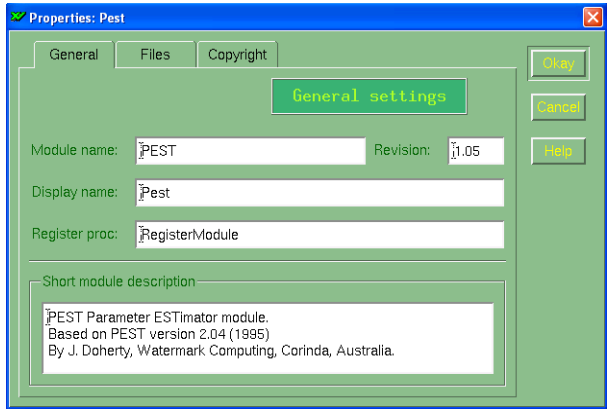


Figure 11.5 Properties dialog.

11.2.4 How to use external modules

11.2.4.1 Interface simulation: attaching a module to a FEM problem

Each module that extends the functionality of a FEM problem will be activated with the 'Select Modules' dialog accessible from the problem editor via the menu entry 'IFM Modules...'. The dialog is shown in Figure 11.6:

All available modules are listed in the left column. Pressing the arrow button activates the selected inactive module. In turn, the IFM attempts to load the DSO (DLL) into memory and to initialize the module. A message box appears should one of these steps fail.

Conversely, a module can be detached by pressing the arrow button for the selected active module. A message box will warn that all module-related data will be lost. Note that as each module is responsible for holding its own data, all such data will be dropped on module detachment.

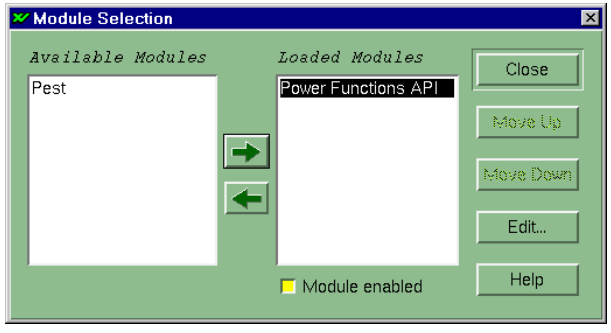


Figure 11.6 Module selection.

The order of the active modules determines the sequence of calling with those at the top of the list being called first. For the operations on a selected *active* module see Table 11.3.

Table 11.3 Operations on an active module

Command	Operation
Move Up	Move the currently selected module one position up. It will be executed before its current predecessor.
Move Down	Move the currently selected active module one position down. It will be executed after its current successor.
Edit...	Edit module-related FEM problem data. This button is only enabled if the module supports, and provides, an appropriate editor for these data.

Private module data can be saved together with the FEM problem by FEFLOW. Whenever FEFLOW detects a module entry while loading a FEM file, it attaches the module automatically and restores the module data.

11.2.4.2 Interface regionalization: database regionalization dialog

Since regionalization can be considered a method applied to FEM-problem data rather than an extension to an FEM problem, modules of the *Regionalization* interface can be activated via graphical interaction elements in the *Database Regionalization Menu*.

If any regionalization modules have been registered a new toggle button appears among the internal regionalization methods. Inverse Distance An option menu allows the selection of the desired module. If the module supports own options you can edit them by pressing the options button Options...; otherwise, the button will be disabled.

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